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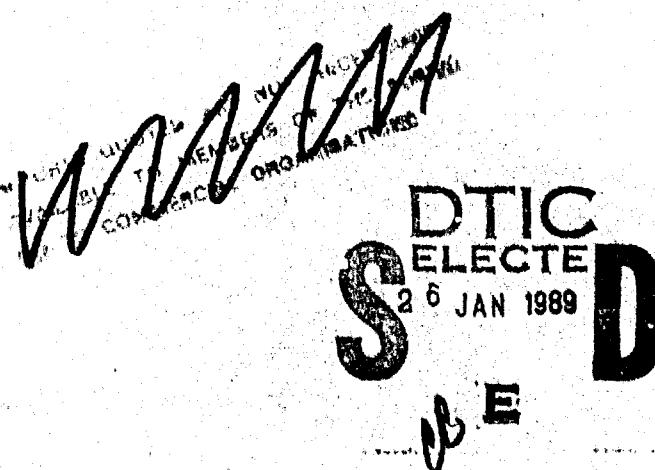
June 1988

**CALCULATION OF THE GLASS
TRANSITION TEMPERATURES OF
LINEAR POLYMERS
PART 3 EVALUATION OF
CALCULATION RELATIONSHIPS**

by

W. A. Lee

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CALCULATION OF THE GLASS TRANSITION TEMPERATURES OF LINEAR POLYMERS PART 3 EVALUATION OF CALCULATION RELATIONSHIPS

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W. A. Lee

SUMMARY

Four equations, relating the structure of polymers in numerical form to their glass transition temperatures (T_g)s, are evaluated using a large data set of 1179 polymers. Additive temperature parameters, for the relationship giving the best fit to the data, are tabulated which enable predictions to be made of many polymer T_g s outside the data set. These parameters also provide a measure of the relative effectiveness of groups in internally plasticising polymers. (P&R - 88-744, JTC)

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1 INTRODUCTION

This is Part 3 of a series of Reports on the calculation of the glass transition temperatures (T_g) of linear polymers. An earlier Technical Memorandum emphasised the importance and significance of the T_g^1 , Part 1 of this series described how a large data set of polymers could be ordered unambiguously², and Part 2 described the data set itself³.

Since the glass transition temperature (T_g) of polymers was first observed, workers have attempted to relate polymer chemical structures to their T_g s and interest in the subject is reflected in the fact that there have been over 100 papers on the calculation of T_g s since 1965. Unfortunately, the polymer data sets to which the relationships have been applied have been insufficiently large, in most cases, to provide an adequate test of their validity; the data chosen could have provided, adventitiously a better fit to the relationships than might be found with a different, or larger, polymer data set. The significance of the size of, and distribution of polymers and groups within, the present data set of 1179 polymers has been discussed³.

In the present Report, the results of applying four relationships to the 1179 polymer data set are described. Additive temperature parameters (ATPs) are calculated which may be used in the prediction of polymer T_g s; these parameters also provide a measure of the relative effectiveness of groups in internally plasticising polymers. This Report goes on to provide analytical data on the results in the form of tables which facilitate updating of the data set by correlating calculation errors with specific polymers and groups. However, this aspect is not pursued in discussion as the main object of this Report is to provide the already-mentioned ATPs.

2 RELATIONSHIPS EVALUATED

Some of the relationships evaluated have been used before on a small data set of polymers having alkyl side chains⁴. A much larger set of such polymers are included in the present data set. The previous analysis did not use the Bayesian statistics of the present calculation and therefore did not provide ATPs for each chemical group as does the treatment described here^{5,6}. There are other distinctions. The relationships tested in the present analysis are:

$$T_g = \sum_{i=1}^{I=x} (n_i T_{g_i}) \quad (1)$$

$$\frac{1}{T_g} = \sum_{i=1}^{I=x} \left(\frac{w_i}{T_{g_i}} \right), \quad (2)$$

and

$$\frac{1}{T_g} = \sum_{i=1}^{i=x} \left(\frac{n_i}{T_{g_i}} \right) , \quad (3)$$

$$\ln T_g = \sum_{i=1}^{i=x} (n_i \ln T_{g_i}) , \quad (4)$$

where T_g = glass transition temperature of the polymer,
 T_{g_i} = the additive temperature parameter (ATP) of the i th group,
 n_i = mole fraction of the i th group,
 w_i = weight fraction of the i th group

and x = the number of groups in the polymer.

In this treatment, a 'group' is considered to be the smallest polymer segment capable of independent torsional oscillation with respect to its nearest neighbours and is otherwise as previously defined³. Each group is identified by an arbitrary code number and the nearest neighbours are considered to be invariant. Dependant as the T_g is on the barriers to rotation between groups and their nearest neighbours, this condition is considered to be an essential aspect of the present treatment. Equation (1) has been successfully applied previously^{7,8} to smaller data sets in a different type of statistical analysis. This equation would be the same as the simplified form of the DiMarzio and Gibbs relationship⁹ if n_i represented the fraction of rotatable (flexible) bonds in the i th group and T_{g_i} were equal to, or a constant fraction of, the T_2 value of a homopolymer of the i th group; T_2 is the temperature below which such a polymer possesses zero configurational entropy. However, the application of the equation here is purely empirical and embodies the assumption that the T_g of a polymer is a linear function of the T_g contributions of its constituent groups in proportion to their mole fractions, with the important qualification, repeated for emphasis, that the neighbours of the single-groups are invariable^{2,3}.

The application of the first equation is illustrated with respect to the first polymer of Table 5 of Part 2³ whose structure, in numerical terms is reproduced below. * indicates the beginning of a new polymer data line, so "833 1" is a continuation line.

* 1 8 219 56 1 57 1 58 1 59 1 60 1 72 2
833 1

The polymer, identified as number 1, contains eight groups, has a T_g of 219 K, has one each of groups type 56, 57, 58, 59, 60 and 833, and two groups of type 72.

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Applying equation (1) we find:

$$219 = (56 + 57 + 58 + 59 + 60 + 72 + 72 + 833)/8 ,$$

where the group numbers, within parentheses, are here used to identify the parameter numbers of groups, (ATPs or Tg_i 's), not the parameter values. Thus, for example, 56 is a parameter number for group 56 which has a value whose units are in degrees K. The Tg is therefore seen to be equated to the average Tg_i (or ATP).

The statistical treatment of the equations is described elsewhere^{5,6}.

3 RESULTS

Each of the equations provided a set of ATPs for the groups in the data set. From these parameters the Tgs of all the polymers were calculated and Table 1 shows the rms of the difference between calculated and observed Tgs (rms) for the four equations.

Table 1

Equation	rms (K)
1	12.6
2	15.6
3	21.1
4	15.2

Evidently, the first equation provides the lowest rms error. The maximum error in calculated Tg (see below) is associated with the same polymer, polymer 1325, for all equations. This polymer has a side-chain of 10 carbon atoms next to a heterocyclic ring and the published Tg may have been accorded to disordering of the carbon chain and be a sub-transition, rather than Tg which is normally regarded as marking substantial rotational liberation in the main chain. However, data have not been excluded from the set unless it was more certain that either the structure of the polymer, or the Tg value were positively in doubt. If the errors in calculated Tg are compared with the polymer structures it will be found that in many instances the higher Tg errors are associated with polymers having long carbon-chain sequences. Table 2 (microfiche) provides details on the difference (DIFF) between observed and estimated Tgs for each polymer using the different equations. In the table, DIFF, FDIFF, HDIFF and LDIFF relate to equations (1) to (4), respectively.

As the lowest errors are associated with equation (1), and equations (1), (3) and (4) are much easier to apply than equation (2), which requires a group

weight parameter, the remainder of this discussion of results is restricted to those deriving from the use of equation (1).

A major interest of the present work stems from the need to know the relative contributions of different groups to the Tgs of polymers. Table 3 therefore shows the ATPs associated with each group in numerical order of increasing ATP and Table 4 presents the same data, but in hierarchical order² of the main (or central) single-group and simultaneously in increasing numerical order of ATP in respect of groups having the same main single-group, but one, or more, different neighbours; main- (M) and side-chain groups (S) are differentiated. This differentiation applies to the central group only. Though it is not the purpose of this Report to do other than present the results in the tables, it will be noted that numerous comparisons may be made between structures and ATPs. In general, despite the empirical nature of the relationships, it is seen that those factors which hinder rotation of the main group with respect to the neighbouring groups, such as polar interaction, bulkiness, steric factors, etc, tend to raise the ATP, and conversely, as is well known for polymer Tgs.

A disturbing feature of the results, despite the low rms error, is the large error in calculated Tg (>20 K) associated with 121 out of 1179 polymers. An analysis is therefore presented showing which polymers are associated with particular calculated Tg errors, Table 5 (microfiche computer printout), and which groups are associated with particular calculated Tg errors, Table 6 (microfiche computer printout). In Table 6, the columns are from left to right: line number (line 1 is not represented), group number, average Tg error (TGE), maximum Tg error, and paired numbers representing polymer number and associated Tg error for however many polymers contained the particular group. Continuation lines are distinguished by having no entries in the second to the fourth columns.

4 CONCLUSIONS

Of four equations, relating the structure of polymers in numerical form to their glass transition temperatures (Tg)s, the best fit, to a large data set of 1179 polymers, is provided by the equation relating the Tg to the mole fraction of groups in the polymers expressed in terms of group additive temperature parameters. An important proviso of the treatment is that the nearest neighbours of groups should be invariant.

Additive temperature parameters, for the relationship giving the best fit to the data, are tabulated which enable predictions to be made of many polymer Tgs outside the data set. These parameters also provide a measure of the relative effectiveness of groups in internally plasticising polymers.

Table 3
GROUPS IN NUMERICAL ORDER OF ATP

162(M) ATP -72	874(M) ATP -52	519(M) ATP 0	773(S) ATP 44
561(M) ATP 52	741(S) ATP 54	1000(M) ATP 58	572(M) ATP 67
691(S) ATP 68	1962(M) ATP 69	1963(M) ATP 69	625(S) ATP 70
548(S) ATP 90	1165(M) ATP 99	546(M) ATP 115	924(S) ATP 115
165(M) ATP 123	163(S) ATP 126	122(M) ATP 127	59(S) ATP 129
643(M) ATP 131	975(M) ATP 132	13(M) ATP 133	236(S) ATP 138
557(S) ATP 138	68(S) ATP 139	49(S) ATP 140	814(S) ATP 147
123(M) ATP 149	508(M) ATP 151	57(S) ATP 153	818(S) ATP 153

$-\text{CH}_2-\text{[CH}_2\text{]}_n-\text{CH}_2-$	$-\text{CH}_2-\overset{\text{CH}_3}{\underset{\text{CH}_3}{\text{Si}}}(\text{CH}_2)$	$-\overset{\text{I}}{\underset{\text{CH}_2}{\text{C}}}-\text{CH}_2-\text{CH}_3$
1321(M) ATP 155	588(M) ATP 157	841(S) ATP 158
$\begin{array}{c} \text{O} \\ \\ \text{CH}_2 \\ \\ \text{CF}_2 \end{array}$	$\begin{array}{c} \text{CH}_2 \\ \\ \text{CH}_2 \\ \\ \text{CF}_3 \end{array}$	$-\overset{\text{Cl}}{\underset{\text{O}}{\text{N}}}=\overset{\text{I}}{\underset{\text{I}}{\text{P}}}-\overset{\text{I}}{\underset{\text{I}}{\text{N}}}=\overset{\text{I}}{\underset{\text{I}}{\text{P}}}-\overset{\text{I}}{\underset{\text{I}}{\text{N}}}=\overset{\text{I}}{\underset{\text{I}}{\text{P}}}-$
181(S) ATP 159	421(S) ATP 159	441(M) ATP 160
$-\text{O}-\text{C}_6\text{H}_4-\text{O}-$	$\begin{array}{c} \text{O} \\ \\ \text{CH}_3-\text{Si}-\text{CH}_3 \\ \\ \text{C}_6\text{H}_5 \end{array}$	$\begin{array}{c} \text{CH}_2 \\ \\ \text{CH}_2 \\ \\ \text{CH}_2 \end{array}$
673(M) ATP 162	951(S) ATP 163	60(S) ATP 164
$-\text{S}-\text{S}-\text{CH}_2-$	$-\overset{\text{I}}{\underset{\text{TRANS}}{\text{C}}}=\text{CH}-\text{CH}_2-\text{CH}_2-$	$\begin{array}{c} \text{I} \\ \\ \text{N} \\ \\ \text{N}=\text{N} \\ \\ \text{C}_6\text{H}_4-\text{NH}- \end{array}$
538(M) ATP 165	849(M) ATP 166	1969(M) ATP 168
$\begin{array}{c} \text{C}_6\text{H}_5 \\ \\ \text{N} \\ \\ \text{C}_6\text{H}_4-\text{N} \\ \\ \text{C}_6\text{H}_4 \end{array}$	$-\overset{\text{I}}{\underset{\text{N}}{\text{C}}}=\overset{\text{O}}{\text{C}}-\text{CH}_2-$	$-\text{N}=\text{PF}_2-\text{N}=\text{PF}_2-\text{N}=\text{PF}_2-$
1970(M) ATP 168	704(M) ATP 169	770(M) ATP 169
$-\text{CH}_2-\text{[CH}_2\text{]}_2-\text{CH}_2-$	$-\text{O}-\text{CH}_2-\overset{\text{I}}{\underset{\text{CH}_2}{\text{C}}}-$	$-\overset{\text{I}}{\underset{\text{CH}_3}{\text{CH}}}=\text{CH}-\overset{\text{I}}{\underset{\text{CH}_2}{\text{CH}}}-\text{CH}_2-$
1302(M) ATP 169	645(M) ATP 170	372(M) ATP 171
$\begin{array}{c} \text{CH}_2 \\ \\ [\text{CH}_2]_4 \\ \\ \text{CH}_2 \end{array}$	$-\text{CH}_2-\text{O}-\text{CH}_2-$	$\begin{array}{c} \text{CH}_2 \\ \\ [\text{CH}_2]_2 \\ \\ \text{CH}_2 \end{array}$
1354(S) ATP 172	99(M) ATP 174	1352(S) ATP 175

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$\begin{array}{c} \text{CH}_2 \\ \\ [\text{CH}_2]_5 \\ \\ \text{CH}_2 \end{array}$	$\begin{array}{c} \text{CH}_2 \\ \\ [\text{CH}_2]_6 \\ \\ \text{CH}_2 \end{array}$
1355(S) RTP 175	1356(S) RTP 175
	$-\text{CF}-\text{O}-\text{CF}_2-$
2058(M) RTP 175	433(M) RTP 177
$-\text{N}-\text{O}-\text{CF}_2-$	$-\text{N}-\text{CF}_2-\text{CF}_2-$
982(M) RTP 177	1076(M) RTP 177
$\begin{array}{c} \text{CH}_3 \\ \\ -\text{O}-\text{Si}-\text{CH}_2- \\ \\ \text{CH}_3 \end{array}$	$-\text{CH}-\text{CH}_2-\text{CH}_2-$
297(M) RTP 181	630(M) RTP 183
$-\text{O}-\text{CH}_2-\text{CF}_2-$	$-\text{O}-\text{CF}_2-\text{CF}_2-$
797(M) RTP 183	26(M) RTP 184
$\begin{array}{c} \text{CH}_2 \\ \\ [\text{CH}_2]_3 \\ \\ \text{CH}_2 \end{array}$	$-\text{CH}_2-\text{CH}(\text{O})-\text{CH}_2-$
1353(S) RTP 184	459(M) RTP 185
$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3-\text{Si}-\text{CH}_3 \\ \\ \text{CH}_3 \end{array}$	$-\text{S}-\text{CF}_2-\text{S}-$
612(S) RTP 185	751(M) RTP 185
$-\text{CH}-\text{O}-\text{CH}_2-$	
471(S) RTP 189	726(S) RTP 191

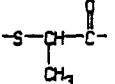
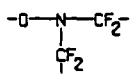
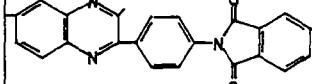
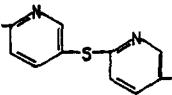
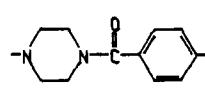
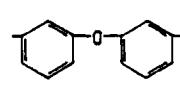
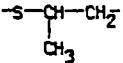
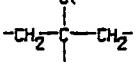
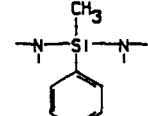
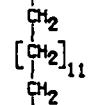
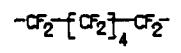
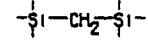
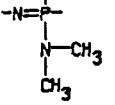
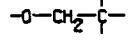
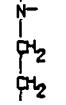
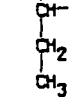
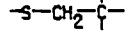
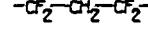
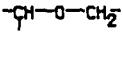
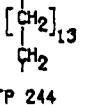
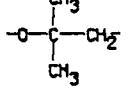
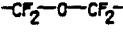
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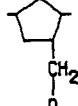
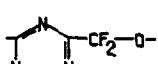
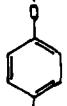
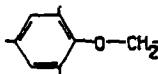
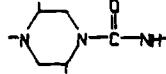
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$-\text{CH}_2-\text{[CH}_2\text{]}_4-\text{CH}_2-$	SYNOIOTACTIC $-\text{CH}_2-\overset{\text{CH}}{\underset{\text{CH}_2}{\text{CH}}}-\text{CH}_2-$	$-\text{O}-\overset{\text{O}}{\underset{\text{I}}{\text{C}}}-\text{CH}-$	$-\text{O}-\text{C}_6\text{H}_4-\text{S}-$
1304(M) RTP 215	531(M) RTP 216	177(M) RTP 218	1112(M) RTP 218
$\begin{array}{c} \text{CF}_2 \\ \\ [\text{CF}_2]_6 \\ \\ \text{CF}_2 \end{array}$	$\begin{array}{c} \text{CF}_2 \\ \\ [\text{CF}_2]_5 \\ \\ \text{CF}_2 \end{array}$	$\begin{array}{c} \text{C}_6\text{H}_5 \\ \\ \text{CH}_3-\text{SI}-\text{CH}_3 \\ \\ \text{O} \end{array}$	$\begin{array}{c} \text{O} \\ \\ \text{CH}_3-\text{SI}-\text{CH}_3 \\ \\ \text{O} \end{array}$
1456(S) RTP 219	1455(S) RTP 221	915(S) RTP 223	929(S) RTP 223
$-\text{CF}-$ O CF_3	$\begin{array}{c} \text{CH}_2 \\ \\ \text{S} \\ \\ \text{CH}_2 \end{array}$	$-\text{CB}_5\text{H}_5\text{C}-\overset{\text{CH}_3}{\underset{\text{CH}_3}{\text{SI}}}-\text{O}-$	$-\text{CH}_2-\text{[CH}_2\text{]}_8-\text{CH}_2-$
48(S) RTP 224	742(S) RTP 225	676(M) RTP 226	1308(M) RTP 226
$-\text{CH}_2-\text{[CH}_2\text{]}_9-\text{CH}_2-$	$-\text{C}(=\text{O})-\text{CH}_2-\overset{\text{I}}{\underset{\text{I}}{\text{CH}}}-$	$-\text{N}=\overset{\text{P}}{\underset{\text{O}}{\text{P}}}-$ C_6H_5	$-\text{CH}_2-\text{CF}_2-\text{CH}_2-$
1309(M) RTP 226	291(M) RTP 227	2212(S) RTP 227	494(M) RTP 228
$-\text{O}-\text{C}_6\text{H}_4-\text{NH}-$	$-\text{CH}-\text{CH}_2-\overset{\text{I}}{\underset{\text{I}}{\text{CH}}}-$	$\begin{array}{c} \text{CH}_2 \\ \\ [\text{CH}_2]_8 \\ \\ \text{CH}_2 \end{array}$	$\begin{array}{c} \text{CH}_3 \\ \\ -\text{O}-\text{SI}-\text{CH}_2 \\ \\ \text{CH}_2 \end{array}$
1237(M) RTP 229	833(M) RTP 230	1358(S) RTP 230	467(M) RTP 231
$-\text{S}-\text{CH}_2-\text{S}-$	$\begin{array}{c} \text{N} \\ \\ \text{CH}-\text{CH}_3 \\ \\ \text{CH}_3 \end{array}$	$-\text{O}-\overset{\text{O}}{\underset{\text{I}}{\text{C}}}-\text{CH}_2-$	$\begin{array}{c} \text{O} \\ \\ \text{CH}-\text{CH}_3 \\ \\ \text{CH}_2 \end{array}$
543(M) RTP 231	1241(S) RTP 231	178(M) RTP 232	237(S) RTP 232
$-\text{CF}_2-\text{[CF}_2\text{]}_6-\text{CF}_2-$	$\begin{array}{c} \text{C=O} \\ \\ \text{O} \\ \\ \text{CH}_2 \end{array}$	$-\text{O}-\text{CH}_2-\text{CH}_2-$	$-\text{O}-\text{C}_6\text{H}_4-\text{CH}_2-$
1406(M) RTP 232	58(S) RTP 233	98(M) RTP 234	651(M) RTP 234

TR 88044

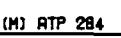
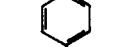
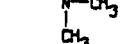
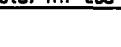
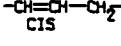
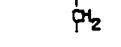
 1910(M) RTP 235	 961(M) RTP 237	 2184(M) RTP 237
 2201(M) RTP 237	 3(M) RTP 238	 454(M) RTP 239
 184(M) RTP 240	 492(M) RTP 240	 608(M) RTP 240
 1361(S) RTP 240	 1404(M) RTP 240	 589(M) RTP 241
 647(S) RTP 241	 846(M) RTP 241	 864(S) RTP 241
 105(S) RTP 242	 555(M) RTP 242	 493(M) RTP 244
 707(M) RTP 244	 1363(S) RTP 244	 231(M) RTP 246
 452(M) RTP 246	 545(M) RTP 246	 609(S) RTP 247

$-CF_2-O-CH_2-$ 159(M) RTP 248		$-CH_2-Si(CH_3)-CH_2-$ 759(M) RTP 249	$-CH_2-CH-CH_2-$ 74(M) RTP 251
$\begin{array}{c} CH \\ \\ CH_2 \\ \\ CH \end{array}$ 334(S) RTP 252		$-CH_2-Si(CH_3)-CH_2-$ 603(M) RTP 252	$\begin{array}{c} CH \\ \\ O \\ \\ CH_2 \end{array}$ 750(S) RTP 253
$-N-CH_2-CH_2-$ 1106(M) RTP 253	$-CF_2-CF-CF_2-$ 55(M) RTP 254	$\begin{array}{c} \text{C=O} \\ \\ \text{C}-\text{O}-\text{C} \end{array}$ 90(M) RTP 254	$\begin{array}{c} \text{N=P} \\ \\ O \\ \\ \text{CH}_3 \end{array}$ 636(S) RTP 254
$-O-CF-CH_2-$ 2055(M) RTP 255	$\begin{array}{c} \text{C=O} \\ \\ -C-CH_2-CH_2- \end{array}$ 14(M) RTP 256	$\begin{array}{c} CF_2 \\ \\ O \\ \\ CF_2 \end{array}$ 259(S) RTP 256	
$\begin{array}{c} CH=CH \\ \\ -C=CH-C(=O) \\ \\ CH_2 \end{array}$ 1164(M) RTP 256	$[CF_2]_4$ 1454(S) RTP 256	$\begin{array}{c} \text{N=P} \\ \\ O \\ \\ \text{C}_6\text{H}_5 \end{array}$ 443(S) RTP 257	$\begin{array}{c} CH \\ \\ CH_2 \\ \\ CH_3 \end{array}$ 554(S) RTP 257
$\begin{array}{c} \text{C=O} \\ \\ -O-CF_2- \end{array}$ 596(M) RTP 257	$\begin{array}{c} \text{C=O} \\ \\ -C-CF_2-CF_2- \end{array}$ 597(M) RTP 257	$\begin{array}{c} CH_2 \\ \\ CH-CH_3 \\ \\ CH_2 \end{array}$ 290(S) RTP 258	$\begin{array}{c} S \\ \\ CH_2 \\ \\ CH_3 \end{array}$ 754(S) RTP 258
 1400(M) RTP 258	$-O-Si(CH_3)-O-$ 266(M) RTP 259	$\begin{array}{c} Br \\ \\ -N=P-N=P-N=P \\ \\ Br \end{array}$ 824(M) RTP 259	$-CH_2-[CH_2]_{12}-CH_2-$ 1312(M) RTP 260
$\begin{array}{c} CF_2 \\ \\ CF_2 \\ \\ CH_2 \end{array}$ 183(S) RTP 263	$-O-Si(CH_3)-\text{C}_6\text{H}_4-$ 710(M) RTP 265		$\begin{array}{c} CF_2 \\ \\ CF_2 \\ \\ NO_2 \end{array}$ 29(S) RTP 266

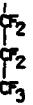
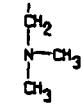
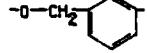
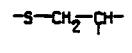
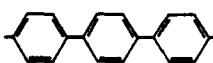
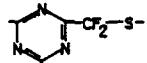
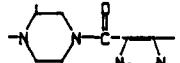
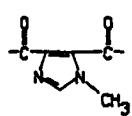
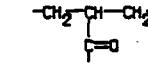
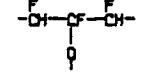
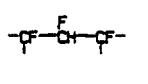
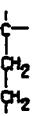
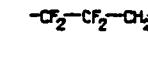
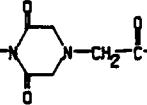
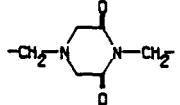
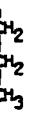
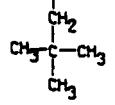
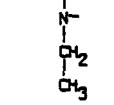
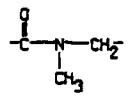
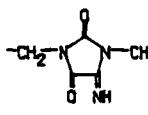
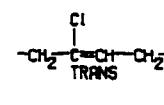
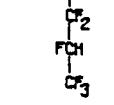
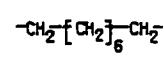
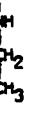
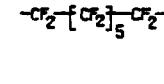
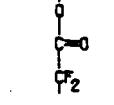
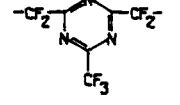
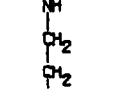
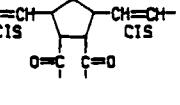
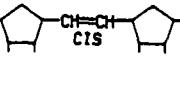
TR 88044

 120(M) RTP 266	 1048(S) RTP 266	 63(S) RTP 267	 1301(M) RTP 267
 84(M) RTP 268	 307(M) RTP 268	 549(S) RTP 270	 251(M) RTP 271
 979(S) RTP 271	 908(M) RTP 271	 1155(M) RTP 271	 1364(S) RTP 271
 84(S) RTP 272	 385(M) RTP 272	 460(M) RTP 273	 497(S) RTP 274
 1053(S) RTP 274	 102(M) RTP 275	 658(M) RTP 275	 153(S) RTP 276
 653(S) RTP 276	 1043(S) RTP 276	 121(M) RTP 277	 594(M) RTP 277
 694(S) RTP 278	 166(S) RTP 279	 431(M) RTP 280	 624(S) RTP 280
 1763(M) RTP 280	 1764(M) RTP 280	 1785(M) RTP 280	 592(M) RTP 281

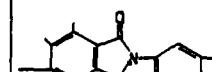
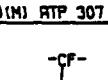
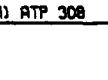
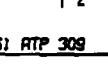
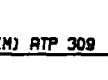
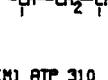
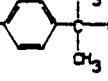
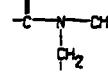
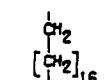
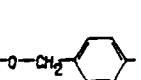
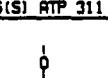
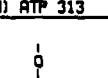
TR 88047

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 239(S) RTP 284	 925(S) RTP 284	 606(S) RTP 285	 716(S) RTP 285
 1365(S) RTP 285	 129(M) RTP 287	 375(M) RTP 288	 377(M) RTP 288
 403(M) RTP 289	 529(M) RTP 289	 847(M) RTP 289	 790(S) RTP 290
 115(M) RTP 291	 442(S) RTP 291	 584(S) RTP 291	 1138(S) RTP 291
 1774(M) RTP 291	 826(S) RTP 292	 933(S) RTP 292	 382(M) RTP 293
 422(S) RTP 293	 436(M) RTP 293	 483(M) RTP 293	 1232(M) RTP 293
 700(S) RTP 295	 1408(M) RTP 295	 1574(S) RTP 295	 468(M) RTP 296

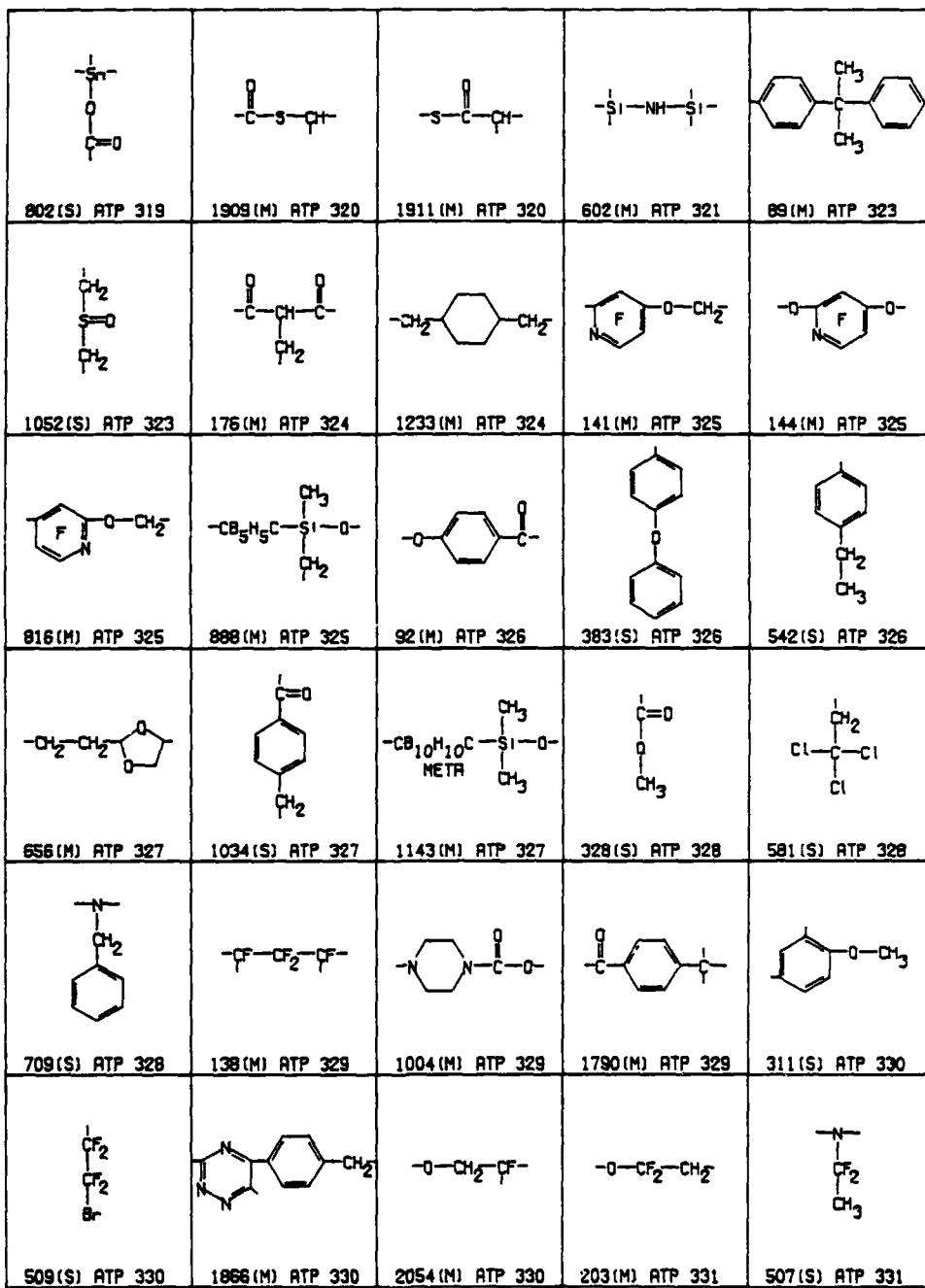
TR 88044

			
768(S) RTP 296	1070(S) RTP 296	43(M) RTP 297	551(M) RTP 297
			
848(S) RTP 297	1531(M) RTP 297	526(M) RTP 298	1925(M) RTP 298
			
1928(M) RTP 298	58(M) RTP 299	132(M) RTP 299	134(M) RTP 299
			
810(S) RTP 299	10(M) RTP 300	1941(M) RTP 300	1942(M) RTP 300
			
72(S) RTP 301	619(S) RTP 301	693(S) RTP 301	706(M) RTP 301
			
1991(M) RTP 301	139(M) RTP 303	778(S) RTP 303	1306(M) RTP 303
			
819(S) RTP 304	1405(M) RTP 304	180(S) RTP 305	595(M) RTP 305
			
752(S) RTP 305	985(S) RTP 305	1162(M) RTP 305	1163(M) RTP 305

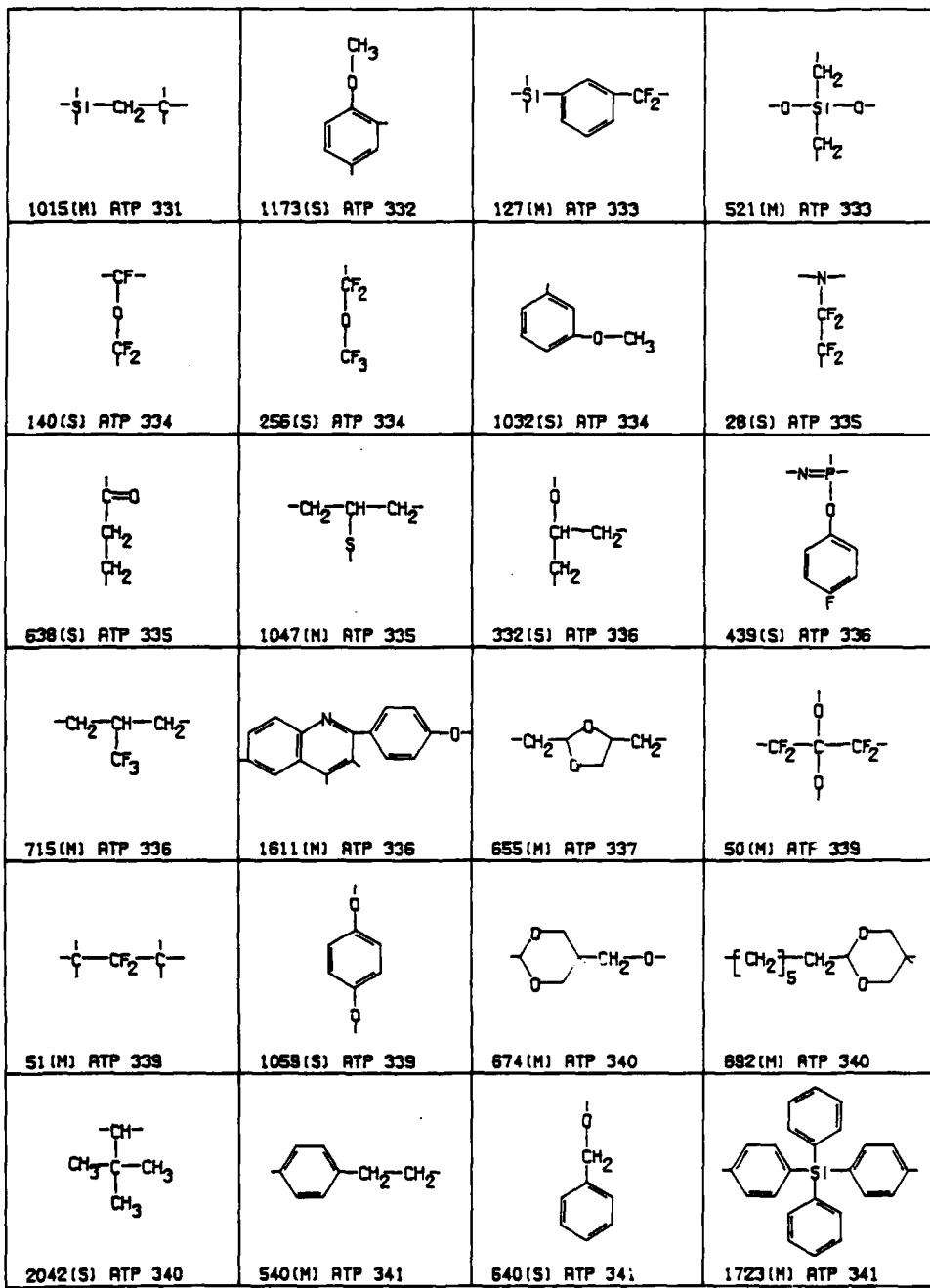
TR. 88044

1170(S) RTP 305	1457(S) RTP 305	583(M) RTP 306	809(M) RTP 306
			
1051(S) RTP 306	638(S) RTP 307	1770(M) RTP 307	44(M) RTP 308
			
131(M) RTP 308	179(S) RTP 308	88(S) RTP 309	135(M) RTP 309
			
138(M) RTP 309	930(M) RTP 309	36(M) RTP 310	535(M) RTP 310
			
621(S) RTP 310	1046(S) RTP 310	646(M) RTP 311	699(M) RTP 311
			
772(S) RTP 311	1135(S) RTP 311	1366(S) RTP 311	46(M) RTP 313
			
223(S) RTP 313	2158(M) RTP 315	783(S) RTP 317	191(S) RTP 319
			
778(S) RTP 318	194(S) RTP 319	263(M) RTP 319	780(S) RTP 319

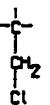
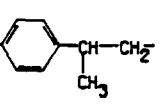
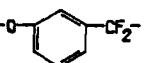
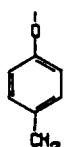
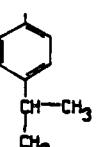
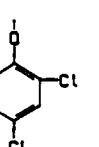
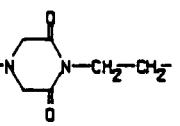
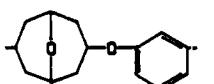
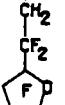
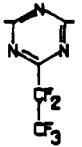
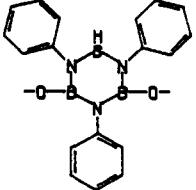
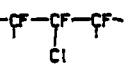
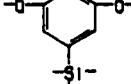
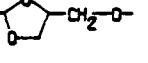
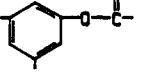
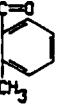
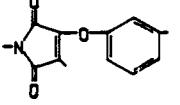
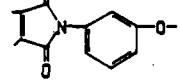
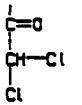
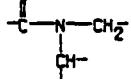
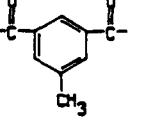
TR 88044



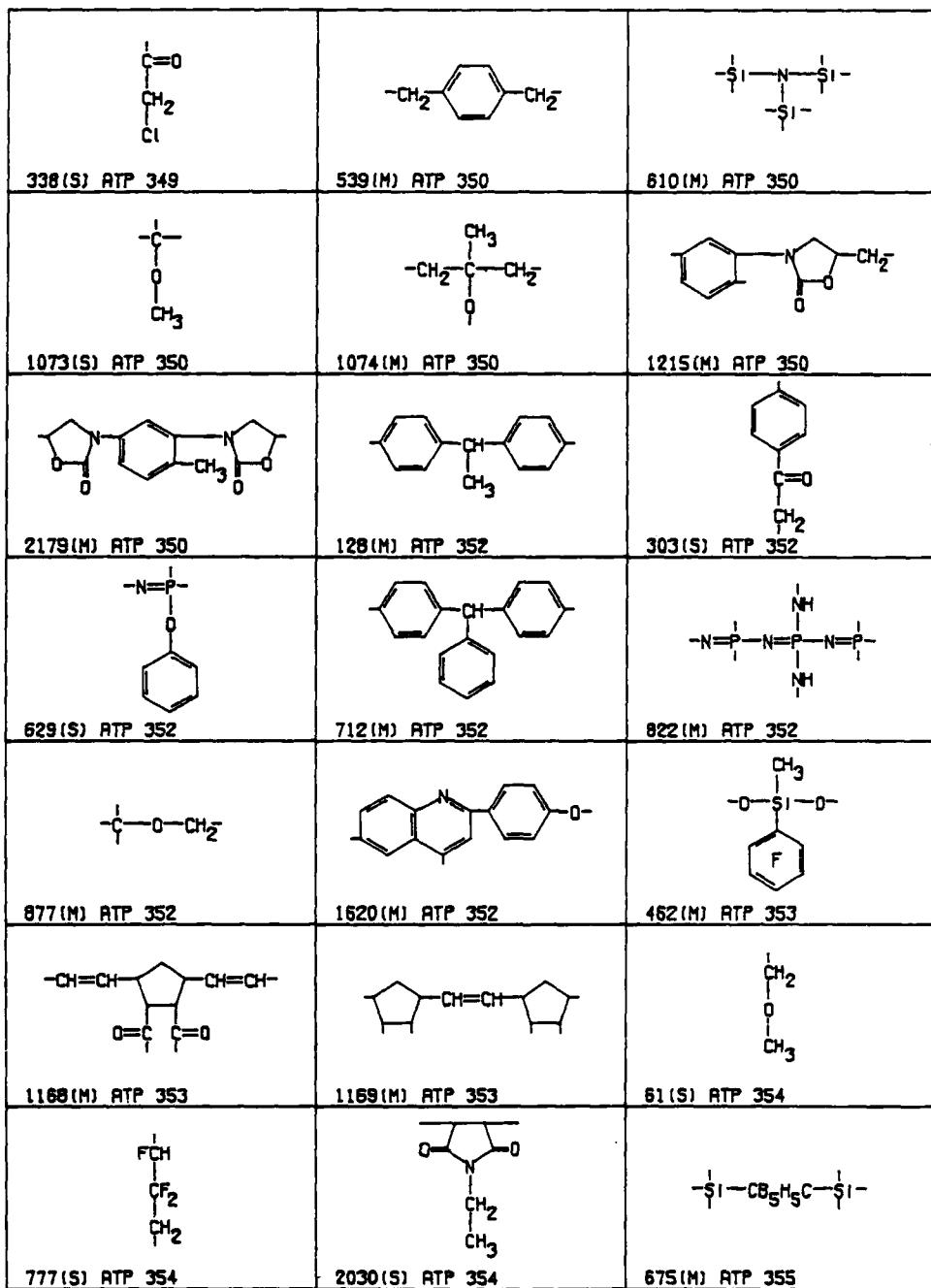
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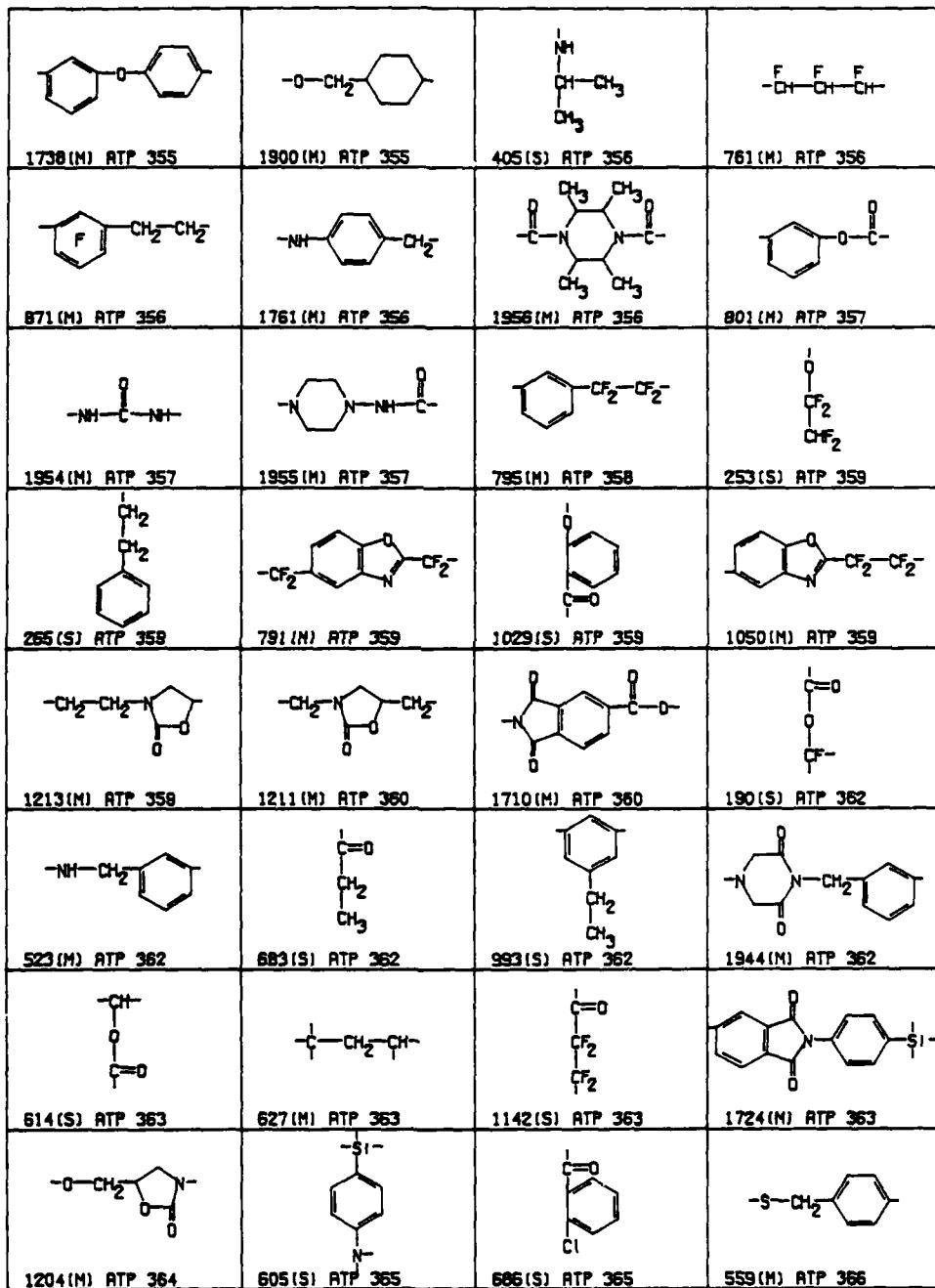
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 2016(M) RTP 343	 470(S) RTP 344	 477(S) RTP 344	 1263(M) RTP 344
 1453(S) RTP 344	 169(M) RTP 345	 905(M) RTP 345	 669(M) RTP 346
 1008(M) RTP 346	 1037(S) RTP 348	 2011(M) RTP 348	 2113(M) RTP 348
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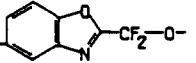
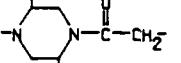
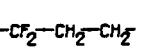
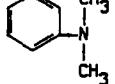
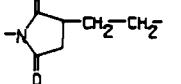
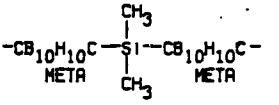
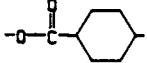
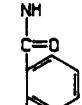
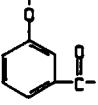
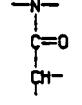
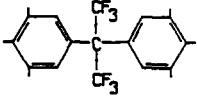
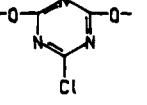
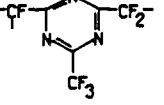
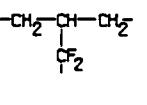
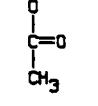
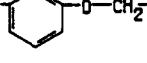
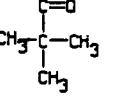
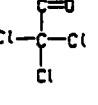
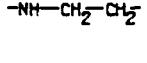
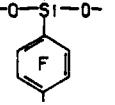
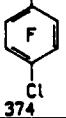
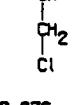
TR 88044



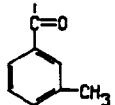
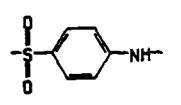
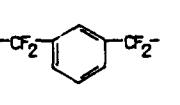
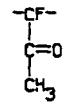
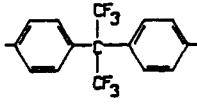
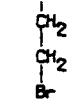
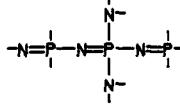
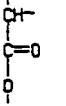
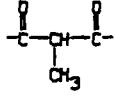
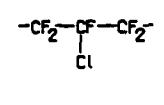
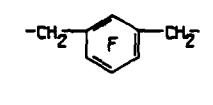
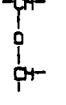
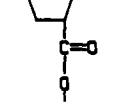
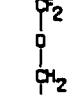
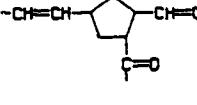
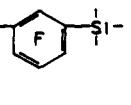
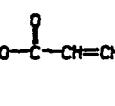
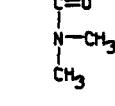
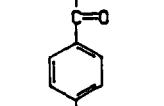
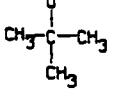
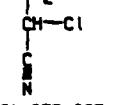
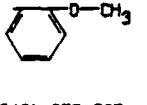
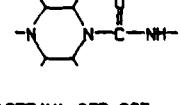
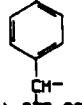
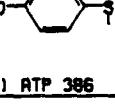
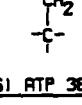
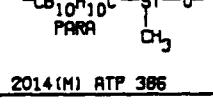
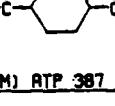
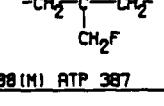
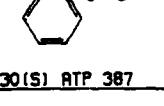
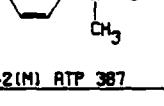
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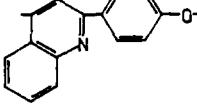
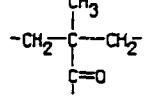
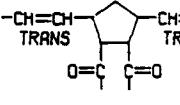
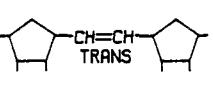
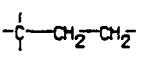
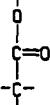
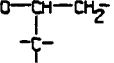
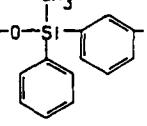
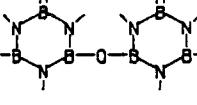
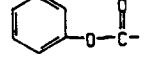
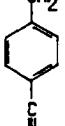
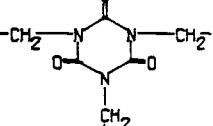
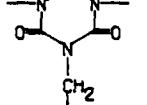
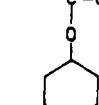
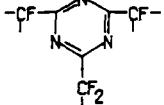
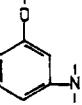
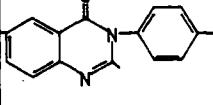
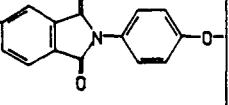
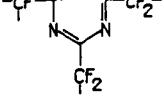
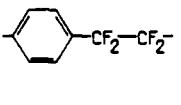
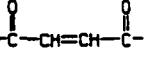
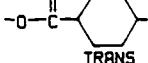
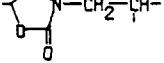
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 1035(S) RTP 366	 1111(M) RTP 366	 1917(M) RTP 366
 469(M) RTP 367	 1065(S) RTP 367	 1993(M) RTP 367
 2013(M) RTP 367	 599(M) RTP 368	 299(S) RTP 369
 1031(S) RTP 369	 1136(S) RTP 369	 2145(M) RTP 370
 1812(M) RTP 371	 528(M) RTP 372	 107(M) RTP 373
 457(S) RTP 373	 541(M) RTP 373	 1021(S) RTP 373
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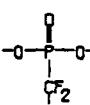
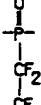
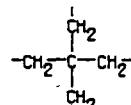
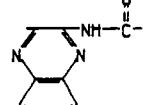
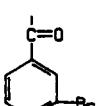
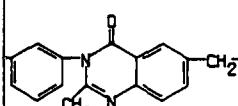
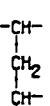
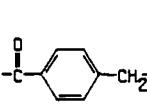
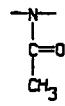
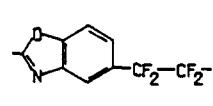
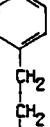
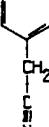
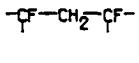
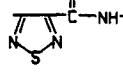
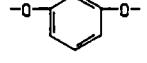
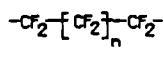
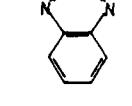
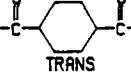
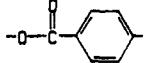
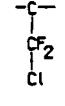
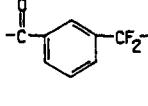
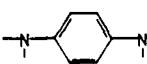
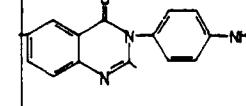
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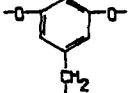
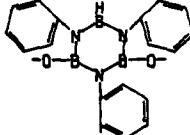
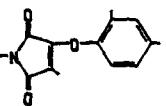
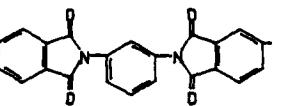
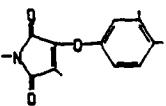
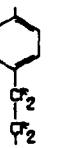
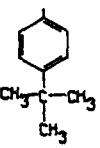
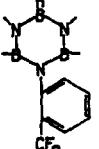
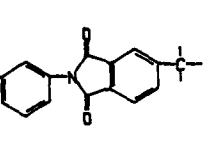
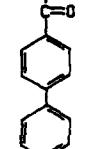
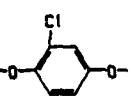
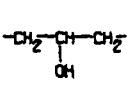
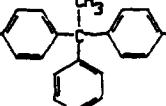
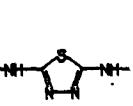
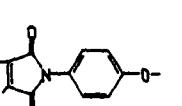
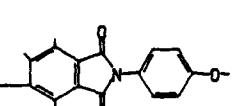
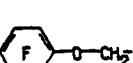
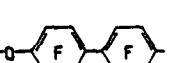
			
1629(M) ATP 388	148(M) ATP 389	689(M) ATP 389	690(M) ATP 389
			
830(M) ATP 389	851(S) ATP 389	973(M) ATP 389	1152(M) ATP 389
			
1261(M) ATP 390	5(S) ATP 391	1061(S) ATP 391	1913(M) ATP 391
			
1914(S) ATP 391	319(S) ATP 392	711(M) ATP 392	1064(S) ATP 392
			
1297(M) ATP 392	1698(M) ATP 392	725(M) ATP 393	997(M) ATP 393
			
591(M) ATP 394	1905(M) ATP 394	2180(M) ATP 394	573(SI) ATP 395

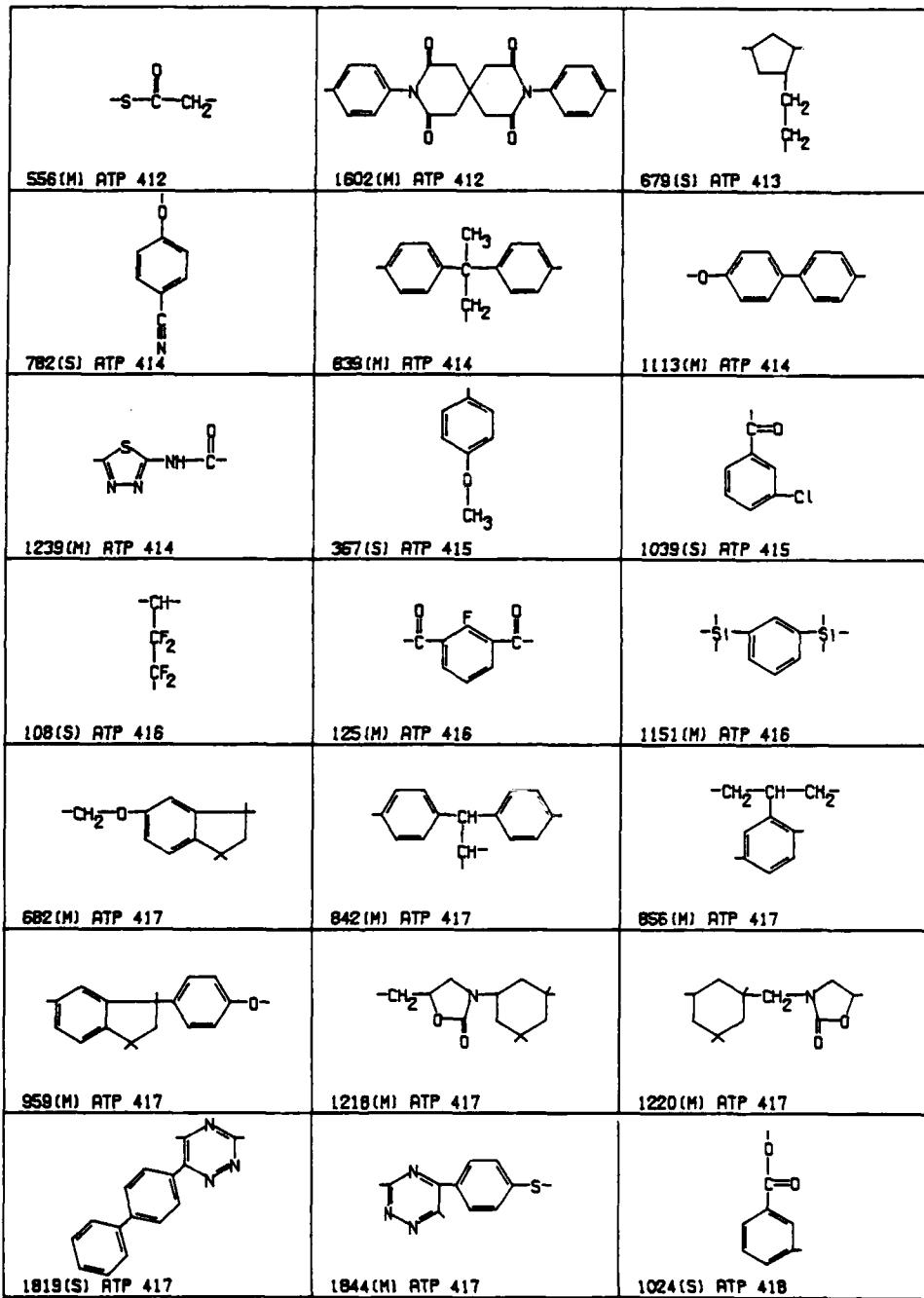
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 1041(S) ATP 396	 1290(M) ATP 396	 2031(S) ATP 396	 93(M) ATP 397
 1133(S) ATP 397	 1063(M) ATP 398	 71(S) ATP 398	 829(S) ATP 399
 1124(M) ATP 399	 1228(M) ATP 399	 903(S) ATP 400	 1071(M) ATP 400
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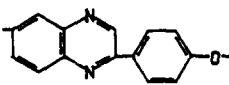
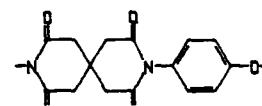
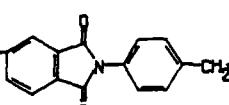
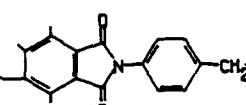
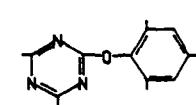
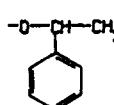
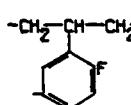
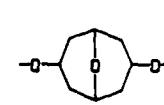
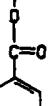
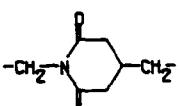
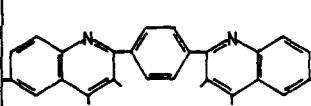
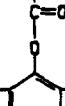
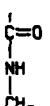
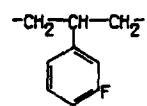
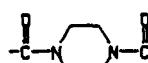
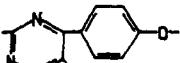
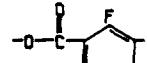
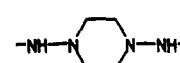
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1257(M) RTP 402	2015(M) RTP 402	724(M) RTP 403
1144(M) RTP 403	171(M) RTP 404	185(S) RTP 404
226(M) RTP 404	232(S) RTP 404	1075(S) RTP 404
1958(M) RTP 404	1959(M) RTP 404	104(M) RTP 405
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1038(S) RTP 405	1740(M) RTP 405	615(S) RTP 406

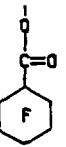
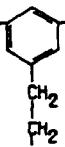
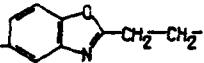
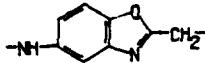
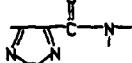
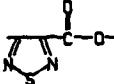
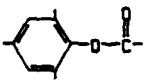
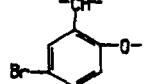
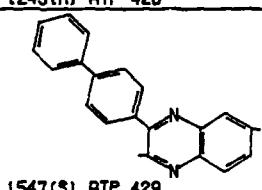
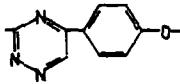
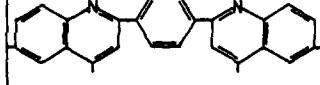
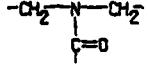
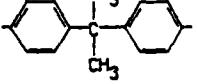
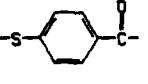
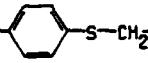
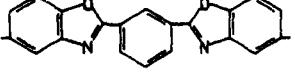
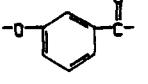
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 2003(M) RTP 406	 2197(M) RTP 406	 2203(M) RTP 406
 113(S) RTP 407	 114(S) RTP 407	 909(S) RTP 407
 1262(S) RTP 407	 1736(M) RTP 407	 1023(S) RTP 408
 2005(M) RTP 408	 503(M) RTP 408	 654(M) RTP 409
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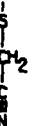
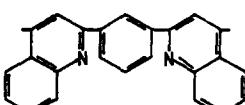
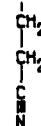
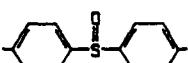
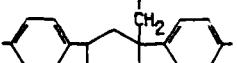
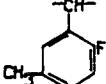
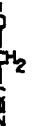
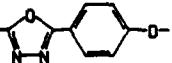
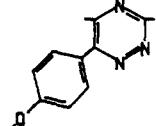
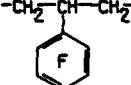
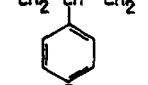
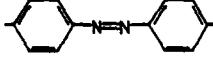
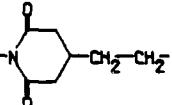
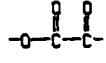
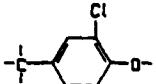
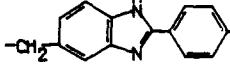
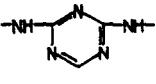
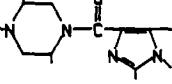
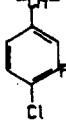


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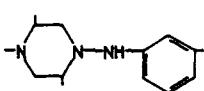
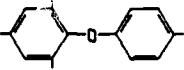
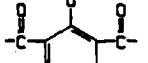
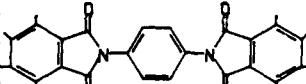
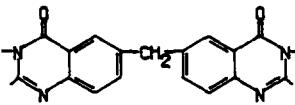
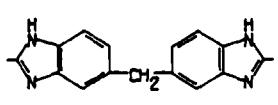
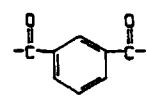
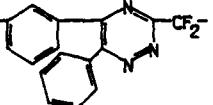
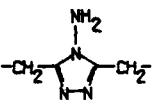
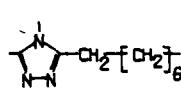
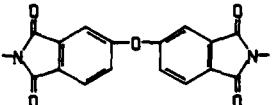
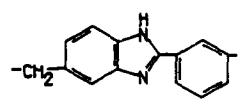
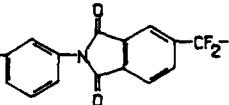
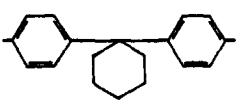
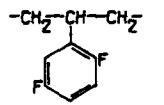
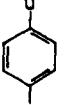
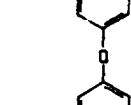
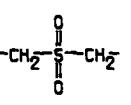
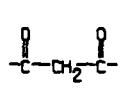
		
1530(M) RTP 419	399(S) RTP 420	1603(M) RTP 420
		
1697(M) RTP 420	1777(M) RTP 420	1855(M) RTP 420
		
708(M) RTP 421	1148(M) RTP 421	1948(M) RTP 421
		
684(S) RTP 422	1966(M) RTP 422	2157(M) RTP 422
		
1056(S) RTP 423	316(S) RTP 424	1149(M) RTP 424
		
438(M) RTP 425	1824(M) RTP 425	126(M) RTP 426
		
1953(M) RTP 426	394(S) RTP 427	660(M) RTP 427

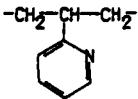
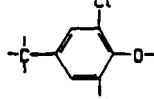
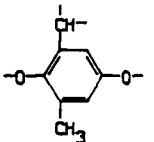
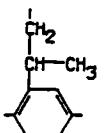
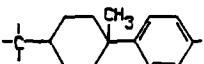
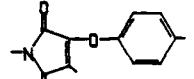
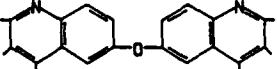
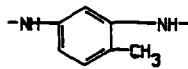
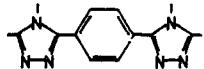
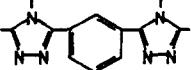
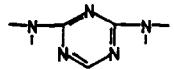
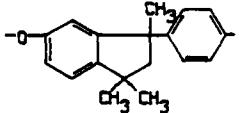
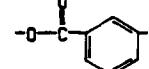
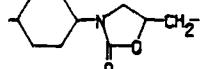
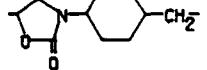
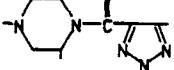
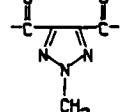
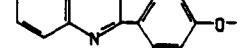
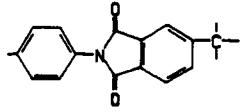
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745(S) RTP 433	2161(M) RTP 433	743(S) RTP 435
		
1108(M) RTP 435	663(M) RTP 436	820(S) RTP 436
		
870(S) RTP 436	1102(M) RTP 436	1817(S) RTP 436
		
2163(M) RTP 436	85(M) RTP 437	1150(M) RTP 437
		
1110(M) RTP 438	1965(M) RTP 438	544(M) RTP 439
		
955(M) RTP 439	419(S) RTP 441	1642(M) RTP 441
		
1695(M) RTP 441	1918(M) RTP 441	355(S) RTP 442

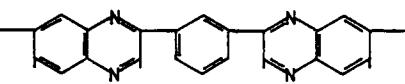
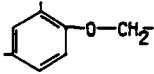
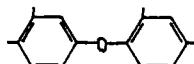
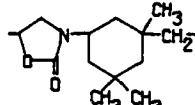
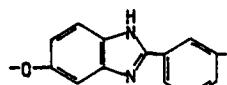
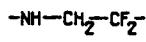
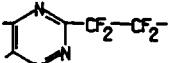
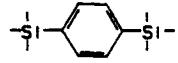
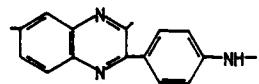
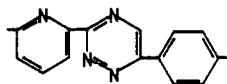
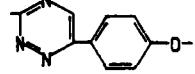
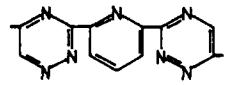
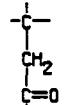
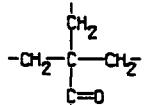
TR 88044

		
1060(S) RTP 442	1937(M) RTP 442	2044(M) RTP 442
		
481(S) RTP 443	490(M) RTP 443	2077(M) RTP 443
		
2154(M) RTP 443	2164(M) RTP 443	243(M) RTP 444
		
1846(M) RTP 444	1967(M) RTP 444	1968(M) RTP 444
		
1156(M) RTP 445	1639(M) RTP 445	1725(M) RTP 445
		
130(M) RTP 446	172(M) RTP 446	628(S) RTP 446
		
1543(S) RTP 446	2047(M) RTP 446	174(M) RTP 447

TR 88044

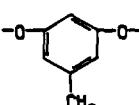
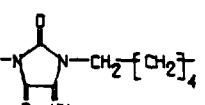
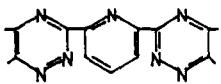
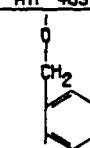
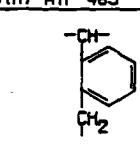
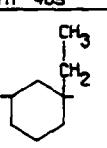
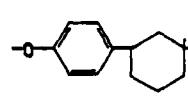
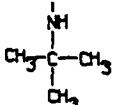
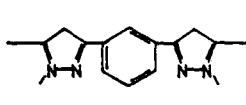
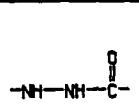
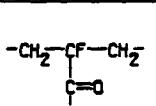
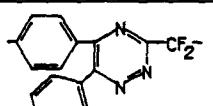
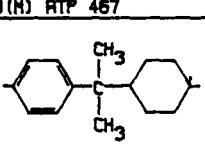
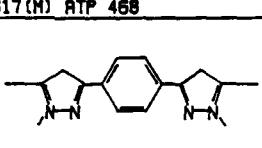
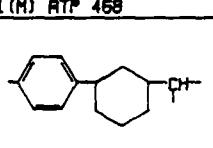
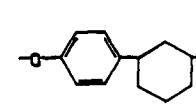
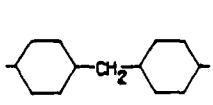
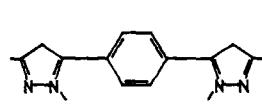
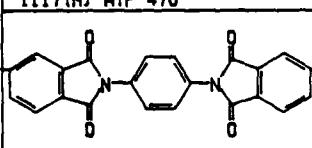
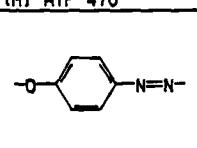
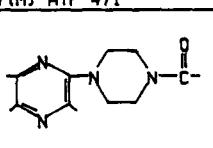
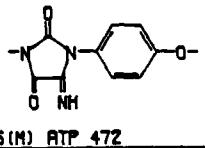
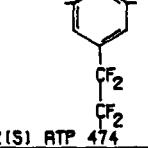
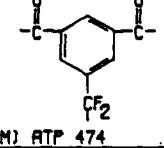
TR 88044

	
2149(M) RTP 453	349(S) RTP 454
	
1161(M) RTP 454	2205(M) RTP 454
	
2206(M) RTP 454	255(S) RTP 455
	
1645(M) RTP 455	197(M) RTP 456
	
1849(M) RTP 456	965(M) RTP 457
	
1573(M) RTP 457	1871(M) RTP 457
	
1872(M) RTP 457	2174(M) RTP 457
	
616(S) RTP 458	807(M) RTP 458

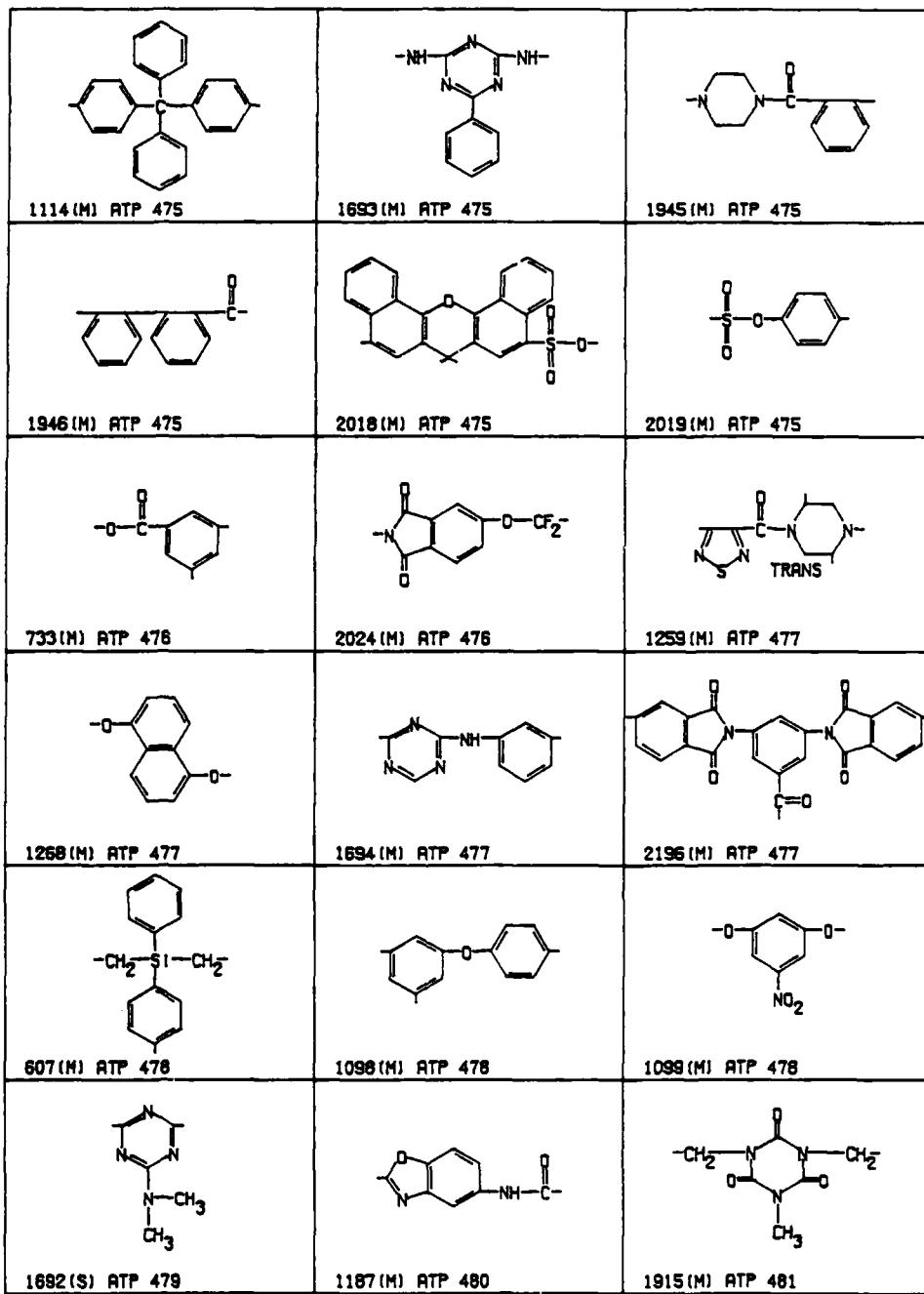
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 860(M) RTP 458	 991(M) RTP 458	 1119(M) RTP 458
 1190(M) RTP 458	 1811(M) RTP 458	 1919(M) RTP 458
 1938(M) RTP 458	 2182(M) RTP 458	 623(S) RTP 459
 2190(M) RTP 459	 667(M) RTP 460	 1634(M) RTP 460
 1141(S) RTP 462	 1600(M) RTP 462	 1676(M) RTP 462
 1677(M) RTP 462	 1992(M) RTP 462	 2123(M) RTP 462
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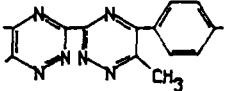
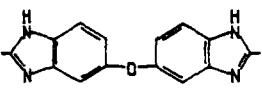
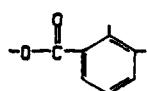
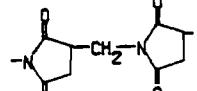
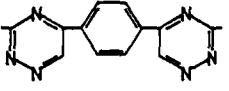
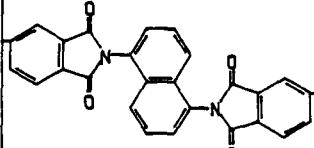
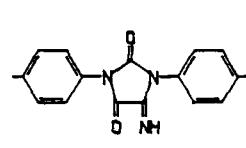
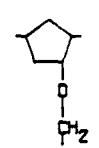
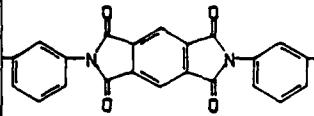
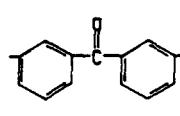
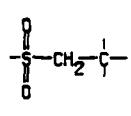
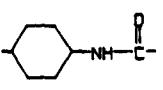
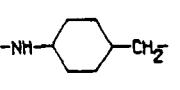
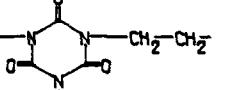
TR 880/4

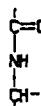
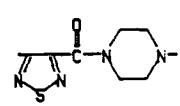
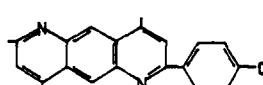
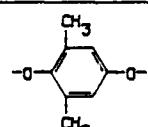
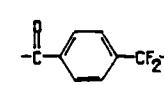
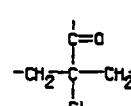
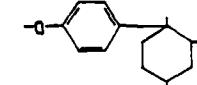
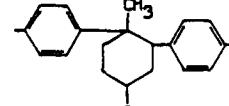
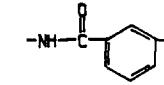
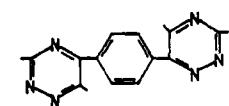
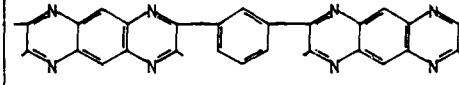
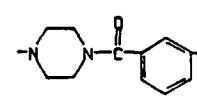
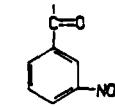
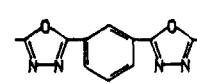
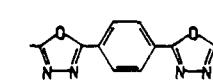
		
		
		
		
		
		
		
		

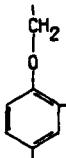
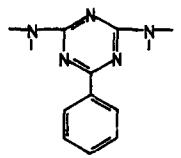
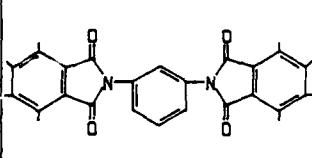
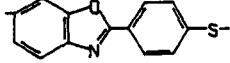
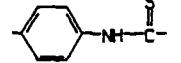
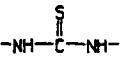
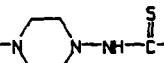
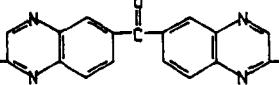
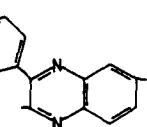
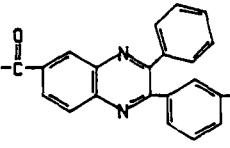
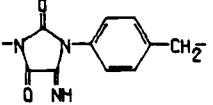
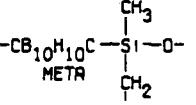
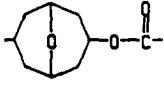
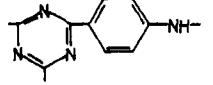
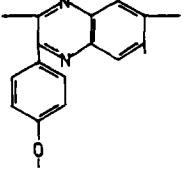
TR 88044



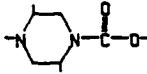
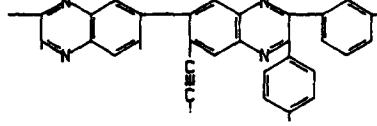
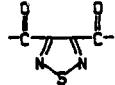
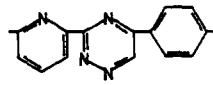
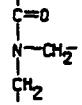
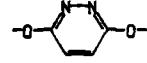
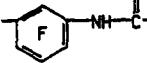
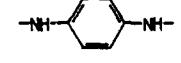
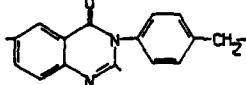
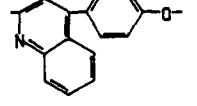
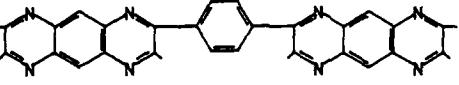
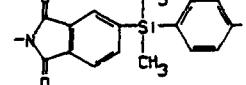
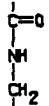
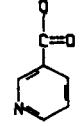
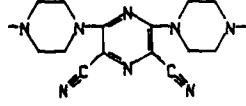
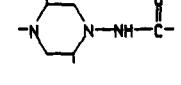
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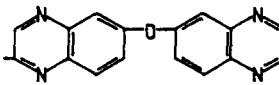
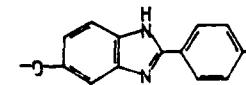
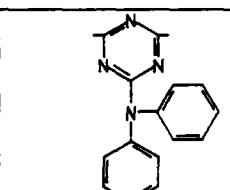
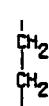
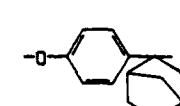
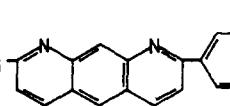
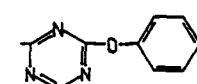
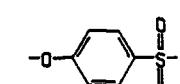
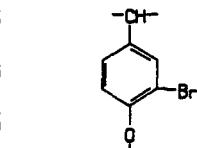
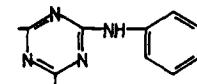
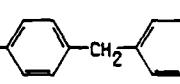
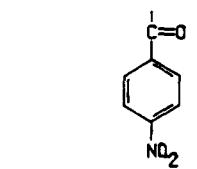
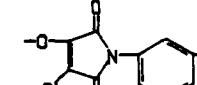
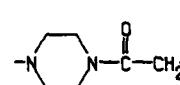
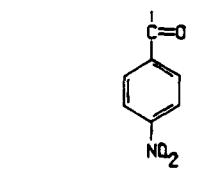
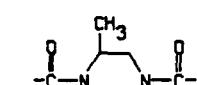
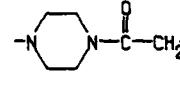
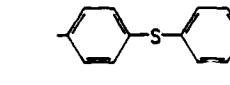
		
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430(N) RTP 482	1068(S) RTP 482	1994(M) RTP 482
		
2131(M) RTP 482	844(S) RTP 483	1137(S) RTP 483
		
2194(M) RTP 483	1986(M) RTP 484	681(S) RTP 485
		
1502(M) RTP 487	1504(M) RTP 487	2046(M) RTP 487
		
1230(M) RTP 488	1231(M) RTP 488	1912(M) RTP 489

	
396(S) RTP 490	1249(M) RTP 490
	
1282(M) RTP 490	2117(M) RTP 490
	
410(S) RTP 491	996(M) RTP 491
	
330(M) RTP 492	668(M) RTP 492
	
953(M) RTP 492	1019(M) RTP 492
	
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1949(M) RTP 493	1025(S) RTP 491
	
1200(M) RTP 494	1202(M) RTP 494

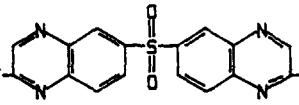
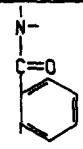
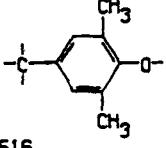
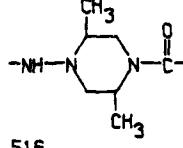
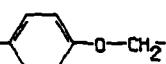
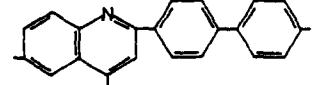
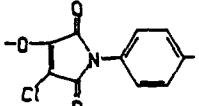
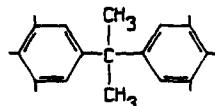
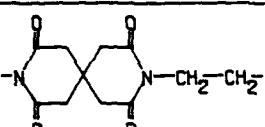
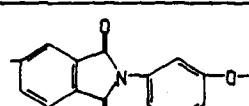
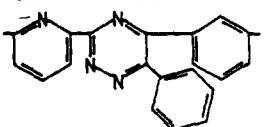
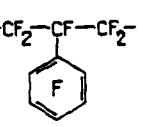
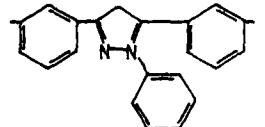
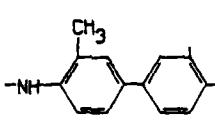
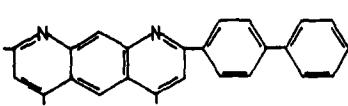
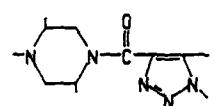
 1174(S) ATP 495	 1859(M) ATP 495	 2078(M) ATP 495
 1196(M) ATP 496	 1950(M) ATP 496	 2048(M) ATP 496
 2052(M) ATP 496	 2152(M) ATP 496	 1542(S) ATP 497
 1580(M) ATP 497	 1987(M) ATP 497	 969(M) ATP 499
 1947(M) ATP 499	 1804(M) ATP 500	 1558(S) ATP 501

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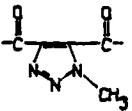
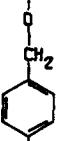
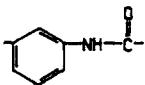
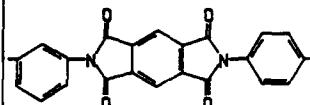
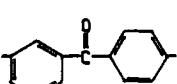
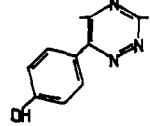
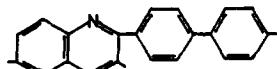
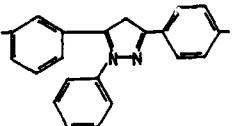
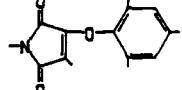
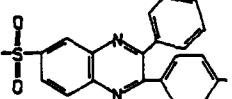
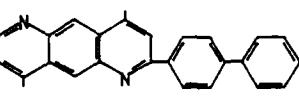
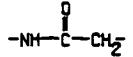
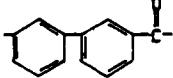
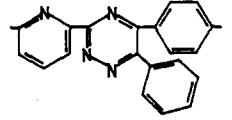
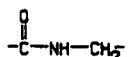
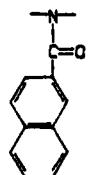
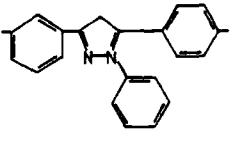
	
1833(M) RTP 501	2148(M) RTP 501
	
1226(M) RTP 502	1867(M) RTP 502
	
400(S) RTP 503	1084(M) RTP 503
	
1153(M) RTP 503	1236(M) RTP 503
	
1295(M) RTP 503	1623(M) RTP 504
	
1274(M) RTP 505	1721(M) RTP 505
	
393(S) RTP 506	910(S) RTP 506
	
1251(M) RTP 506	1939(M) RTP 506

		
2185(M) ATP 506	1648(M) ATP 508	1671(S) ATP 508
		
748(S) RTP 509	1118(M) ATP 510	1283(M) ATP 510
		
1813(M) ATP 510	666(M) ATP 511	1172(S) RTP 511
		
1690(M) ATP 511	96(M) ATP 512	1027(S) RTP 512
		
2008(M) ATP 512	437(M) ATP 513	641(M) ATP 513
		
1258(M) ATP 513	1553(S) ATP 513	1057(S) RTP 514

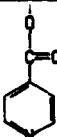
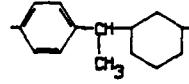
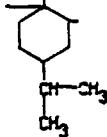
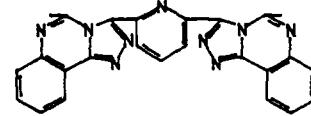
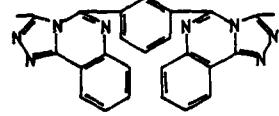
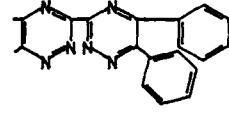
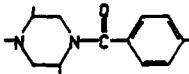
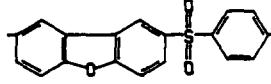
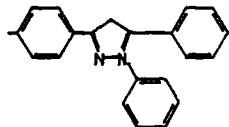
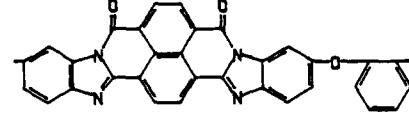
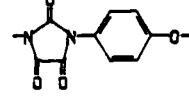
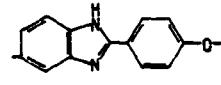
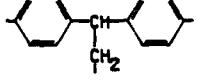
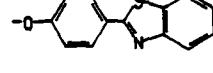
TR 88044

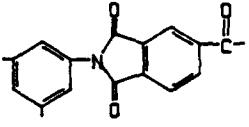
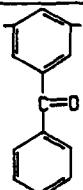
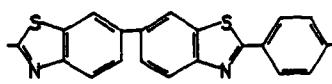
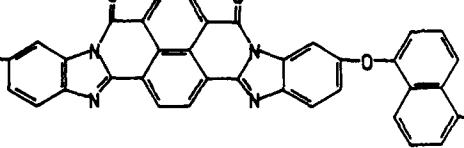
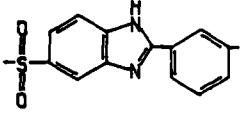
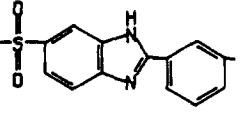
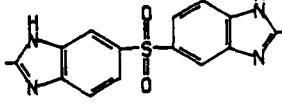
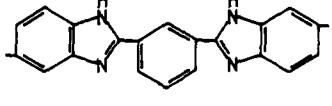
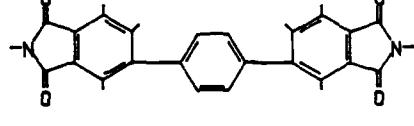
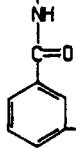
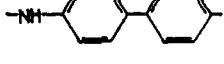
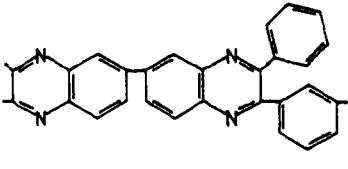
	
2186(M) ATP 514	296(S) ATP 516
	
1096(M) ATP 516	1936(M) ATP 516
	
97(M) ATP 517	1617(M) ATP 517
	
1999(M) ATP 517	2089(M) ATP 517
	
1601(M) ATP 518	1727(M) ATP 518
	
1860(M) ATP 518	195(M) ATP 519
	
1973(M) ATP 520	2133(M) ATP 520
	
1281(M) ATP 523	1927(M) ATP 524

TR 88044

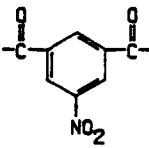
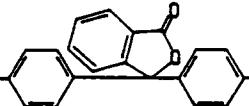
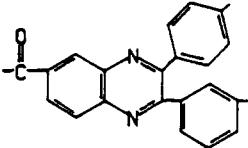
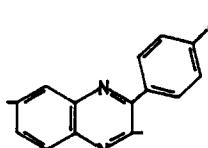
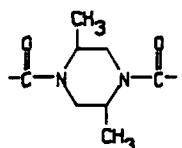
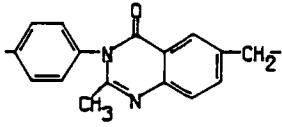
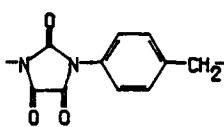
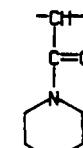
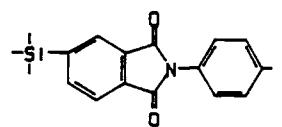
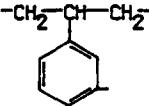
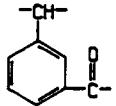
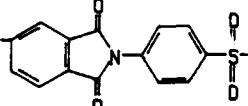
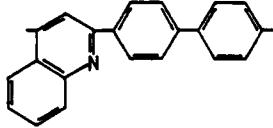
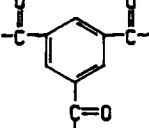
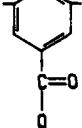
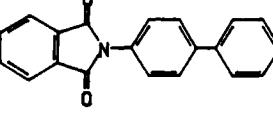
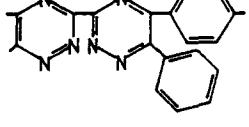
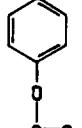
TR 88044

 986(S) RTP 535	 1115(M) RTP 535
 671(S) RTP 536	 2148(M) RTP 536
 2207(H) RTP 536	 2167(M) RTP 537
 1940(M) RTP 538	 2049(M) RTP 538
 1976(M) RTP 540	 1265(M) RTP 541
 1288(M) RTP 541	 1981(M) RTP 541
 2130(M) RTP 541	 1644(M) RTP 544
 843(M) RTP 547	 1225(M) RTP 548

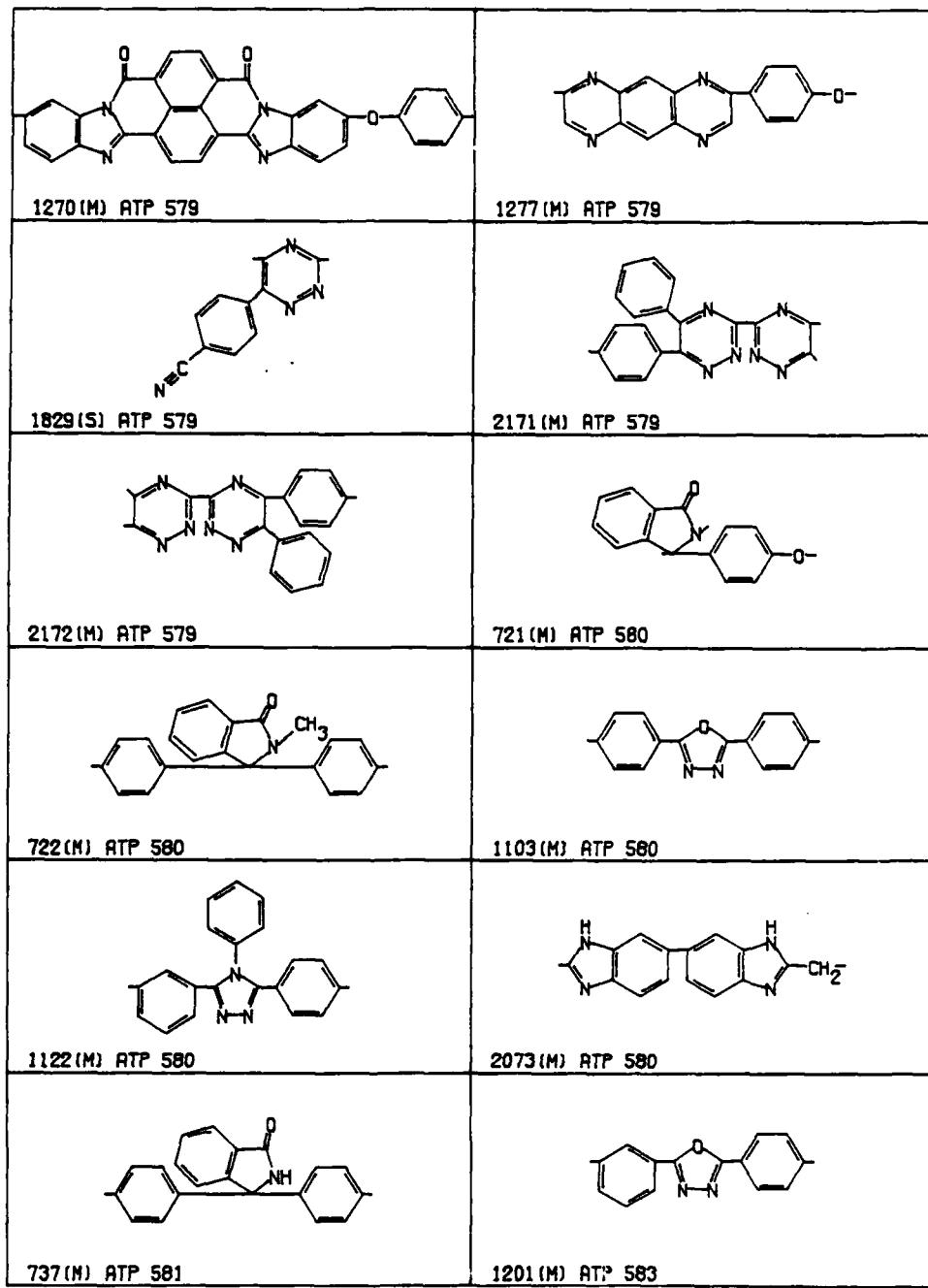
	
1681(M) ATP 548	1683(S) ATP 548
	
2143(M) ATP 548	1267(M) ATP 549
	
1650(M) ATP 549	2175(M) ATP 549
	
2176(M) ATP 549	2178(M) ATP 549
	
2192(M) ATP 550	1175(S) ATP 551
	
1678(M) ATP 551	2166(M) ATP 551

TR 88044

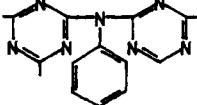
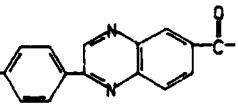
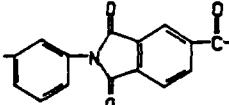
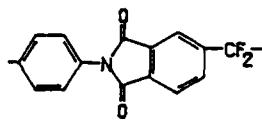
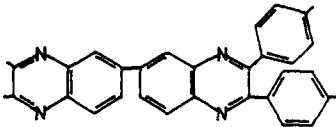
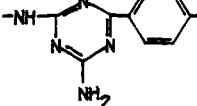
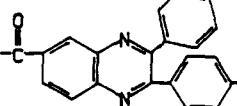
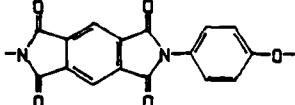
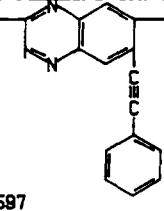
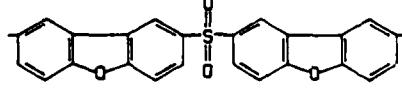
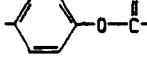
TR 88044

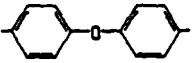
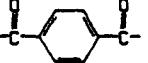
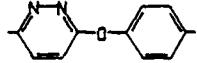
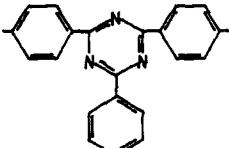
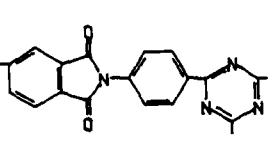
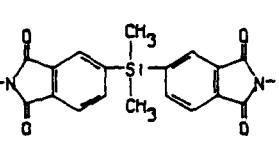
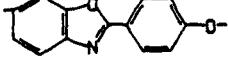
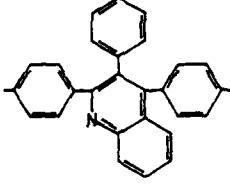
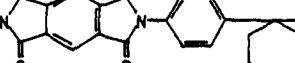
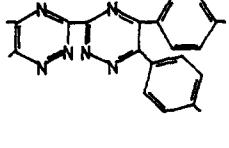
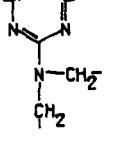
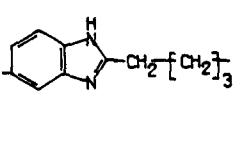
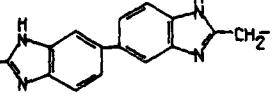
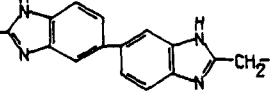
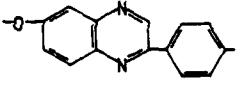
 1906(M) ATP 563	 730(M) ATP 565	 1540(M) ATP 565
 1544(S) ATP 565	 1916(M) ATP 565	 1293(M) ATP 566
 1979(M) ATP 566	 408(S) ATP 567	 1717(M) ATP 569
 904(M) ATP 571	 1171(S) ATP 571	 1703(M) ATP 571
 1633(M) ATP 575	 1581(M) ATP 576	 1582(S) ATP 576
 1679(M) ATP 577	 2126(M) ATP 578	 781(S) ATP 579

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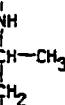
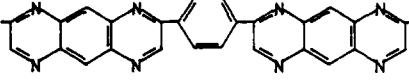
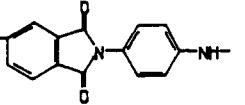
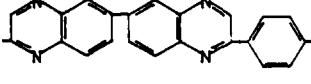
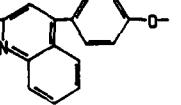
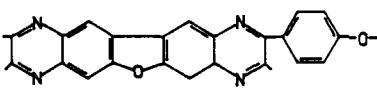
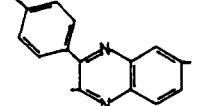
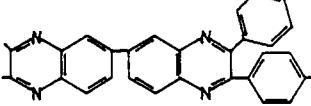
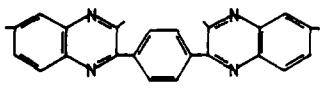
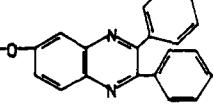
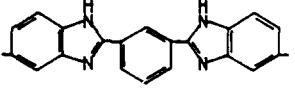
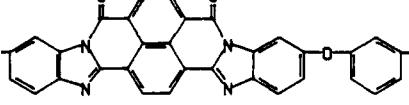
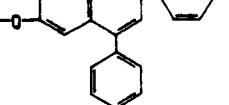
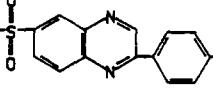


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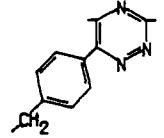
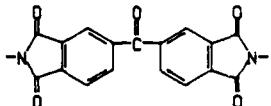
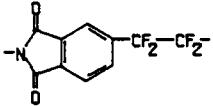
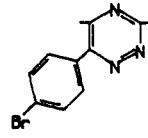
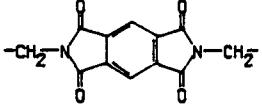
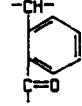
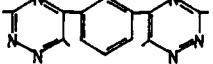
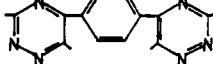
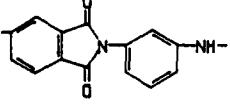
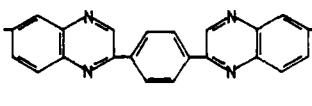
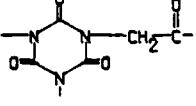
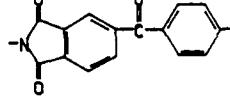
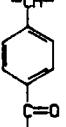
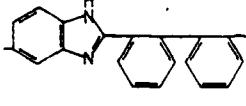
	
1858(M) ATP 584	1591(M) ATP 586
	
1086(M) ATP 589	698(S) ATP 590
	
2040(M) ATP 590	2150(M) ATP 591
	
1803(M) ATP 595	1578(M) ATP 596
	
1513(M) ATP 597	1559(S) ATP 597
	
1878(M) ATP 597	109(M) ATP 599

		
100(M) ATP 600	142(M) ATP 600	1093(M) ATP 600
		
1700(M) ATP 600	1701(M) ATP 600	2193(M) ATP 600
		
1194(M) ATP 602	1621(M) ATP 602	1508(M) ATP 605
		
2127(M) ATP 605	1663(S) ATP 606	2111(M) ATP 606
		
2210(M) ATP 606	2211(M) ATP 606	1594(M) ATP 607

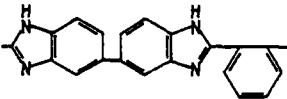
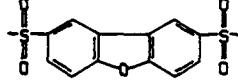
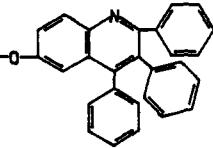
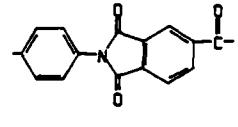
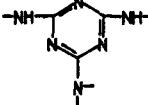
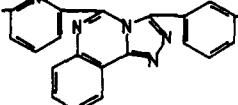
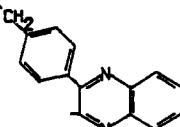
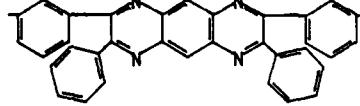
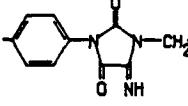
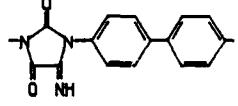
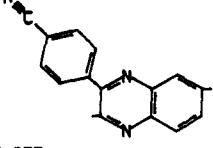
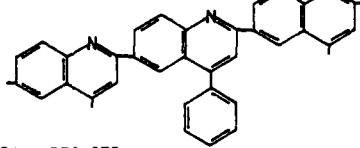
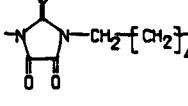
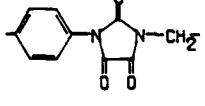
TR 88044

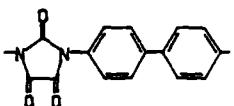
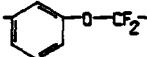
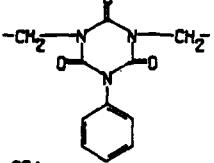
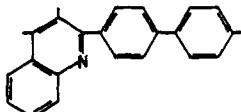
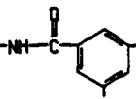
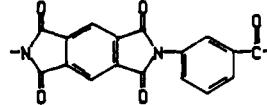
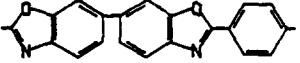
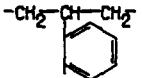
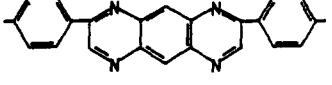
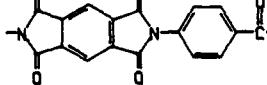
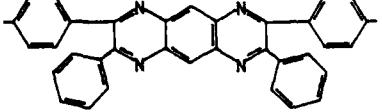
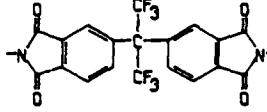
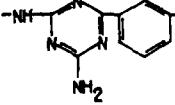
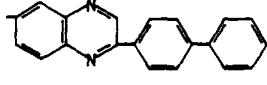
	
395(S) RTP 608	1276(M) RTP 608
	
1760(M) RTP 608	2051(M) RTP 609
	
1630(M) RTP 613	1181(M) RTP 614
	
1536(S) RTP 616	2067(M) RTP 616
	
2068(M) RTP 616	1583(M) RTP 617
	
2163(M) RTP 617	1269(M) RTP 620
	
1613(M) RTP 621	1597(M) RTP 624

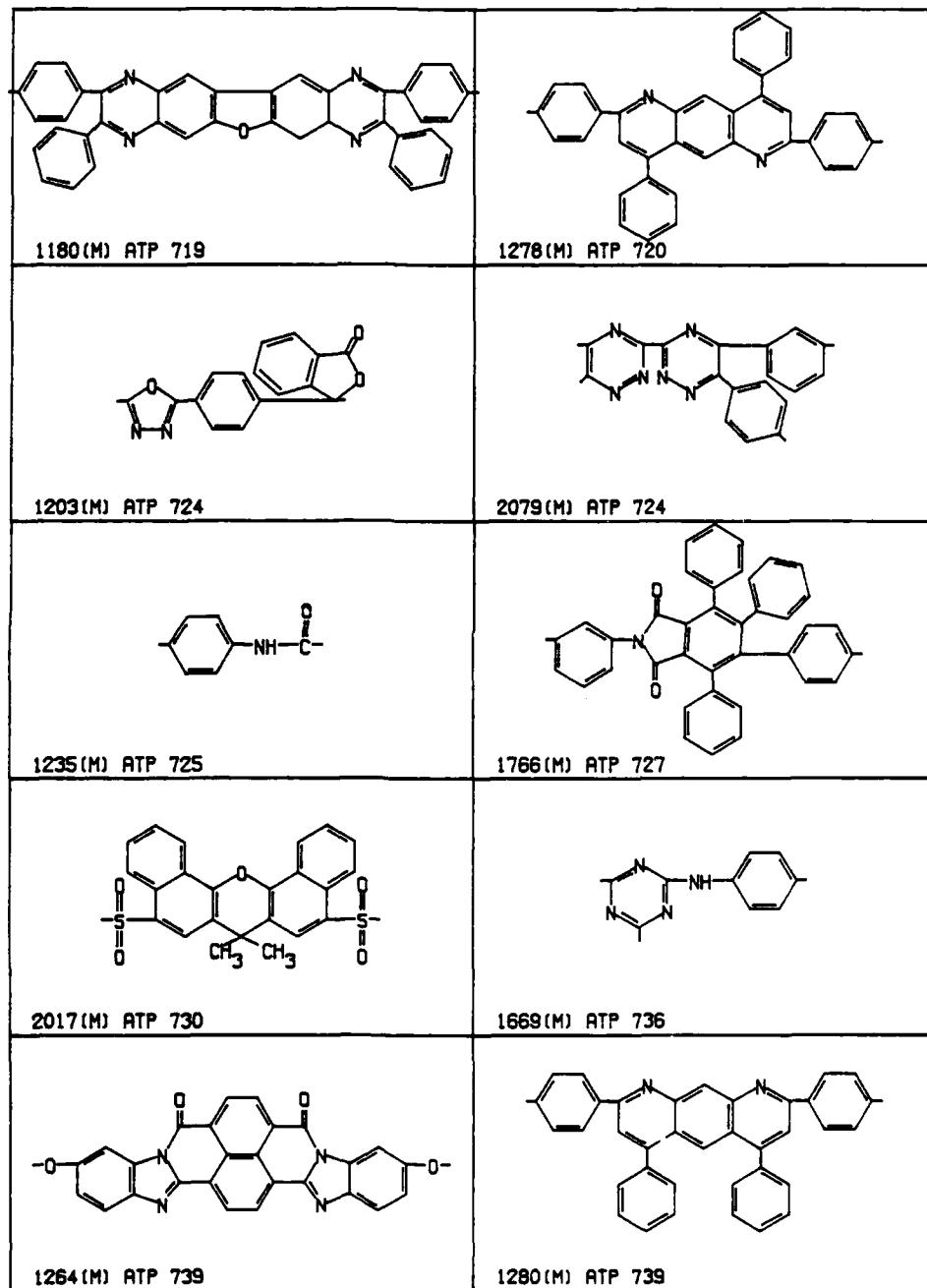
TR 88044

	
1827(S) RTP 627	1085(M) RTP 628
	
1006(M) RTP 630	1825(S) RTP 631
	
1299(M) RTP 633	272(S) RTP 635
	
2080(M) RTP 635	2081(M) RTP 637
	
1691(M) RTP 642	2062(M) RTP 645
	
1874(M) RTP 647	2075(M) RTP 648
	
960(S) RTP 651	1780(M) RTP 659

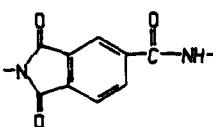
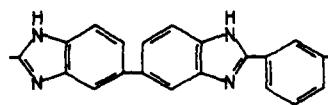
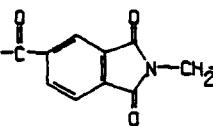
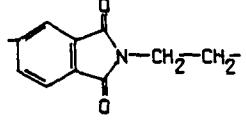
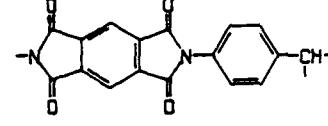
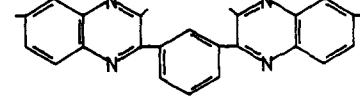
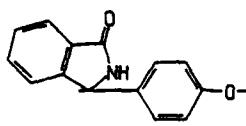
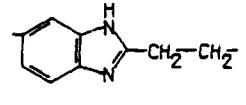
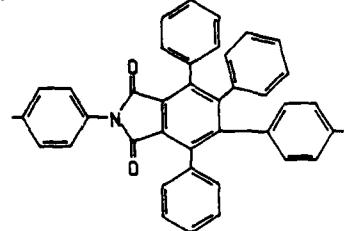
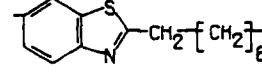
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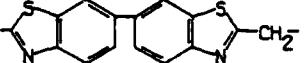
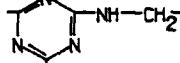
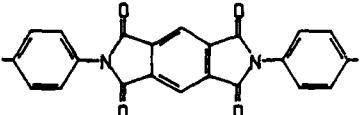
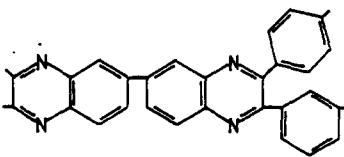
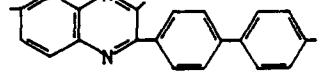
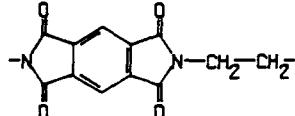
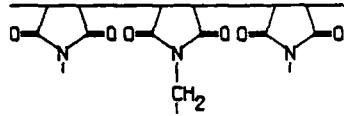
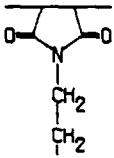
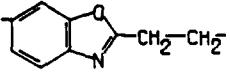
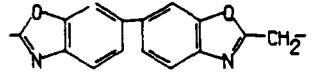
	
2165(M) RTP 659	1879(M) RTP 663
	
1604(M) RTP 664	1084(M) RTP 665
	
1661(M) RTP 665	1287(M) RTP 666
	
1549(S) RTP 666	1271(M) RTP 668
	
1989(M) RTP 673	1990(M) RTP 673
	
1551(S) RTP 675	1612(M) RTP 676
	
1982(M) RTP 678	1983(M) RTP 678

	
1984(M) RTP 678	1726(M) RTP 684
	
1873(M) RTP 684	1626(M) RTP 685
	
1016(M) RTP 690	1503(M) RTP 690
	
2060(M) RTP 693	373(M) RTP 695
	
1275(M) RTP 695	1507(M) RTP 695
	
1273(M) RTP 705	2074(M) RTP 713
	
1800(M) RTP 714	1527(M) RTP 717



TR 88044

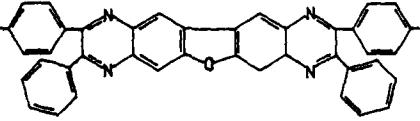
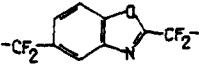
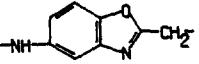
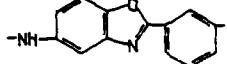
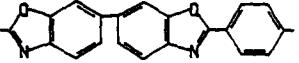
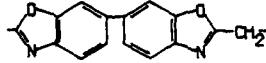
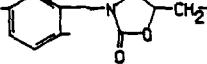
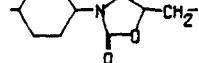
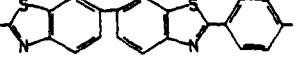
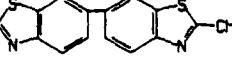
	
1702(M) ATP 740	2168(M) ATP 740
	
1708(M) ATP 741	1714(M) ATP 741
	
1501(M) ATP 753	2066(M) ATP 755
	
738(M) ATP 758	1673(M) ATP 781
	
1772(M) ATP 783	2093(M) ATP 787

	
2144(M) ATP 787	1660(M) ATP 806
	
1500(M) ATP 823	2065(M) ATP 825
	
1565(M) ATP 837	1298(M) ATP 861
	
1781(M) ATP 865	1783(S) ATP 891
	
1197(M) ATP 1043	2139(M) ATP 1043

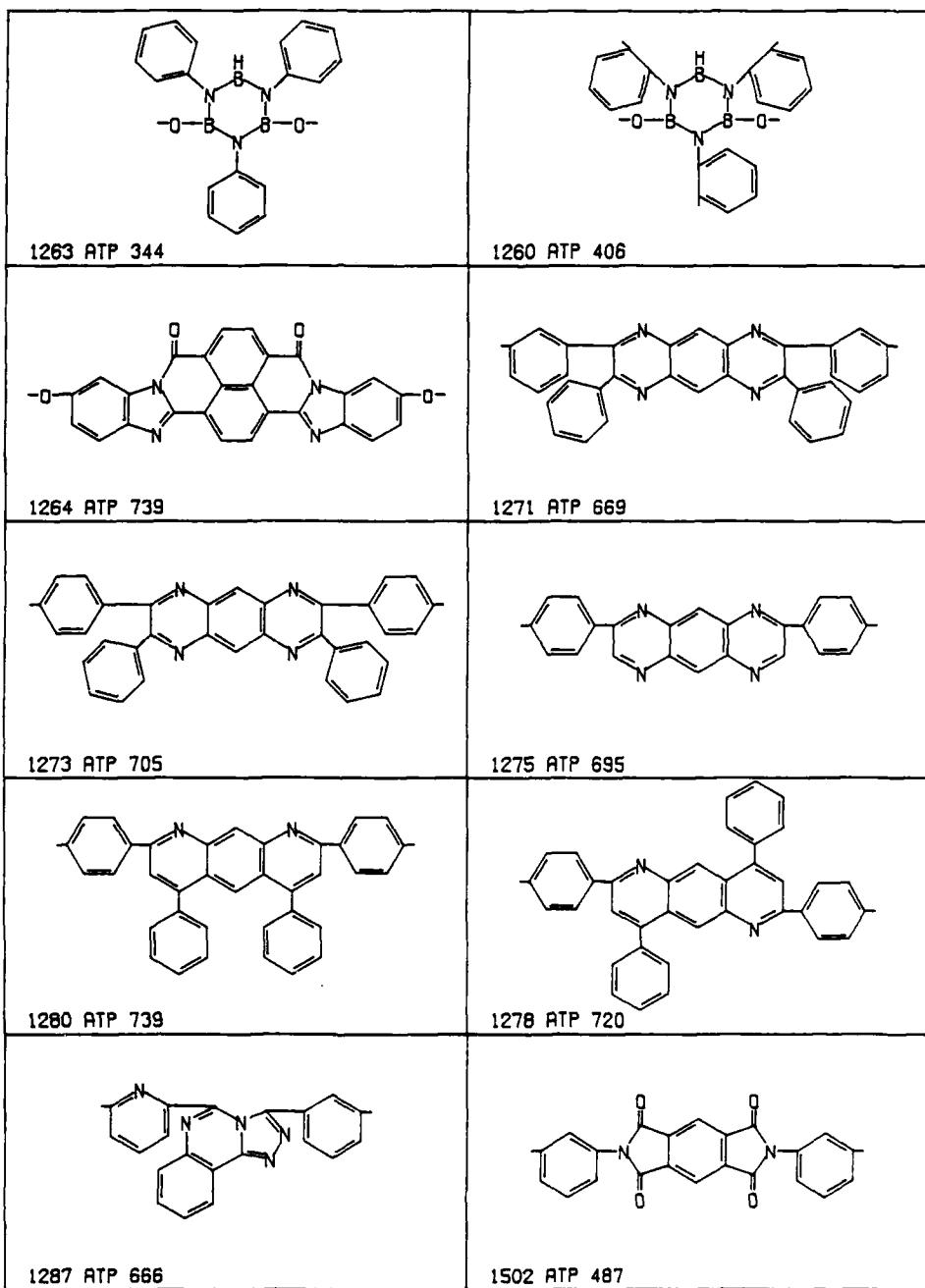
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Table 4

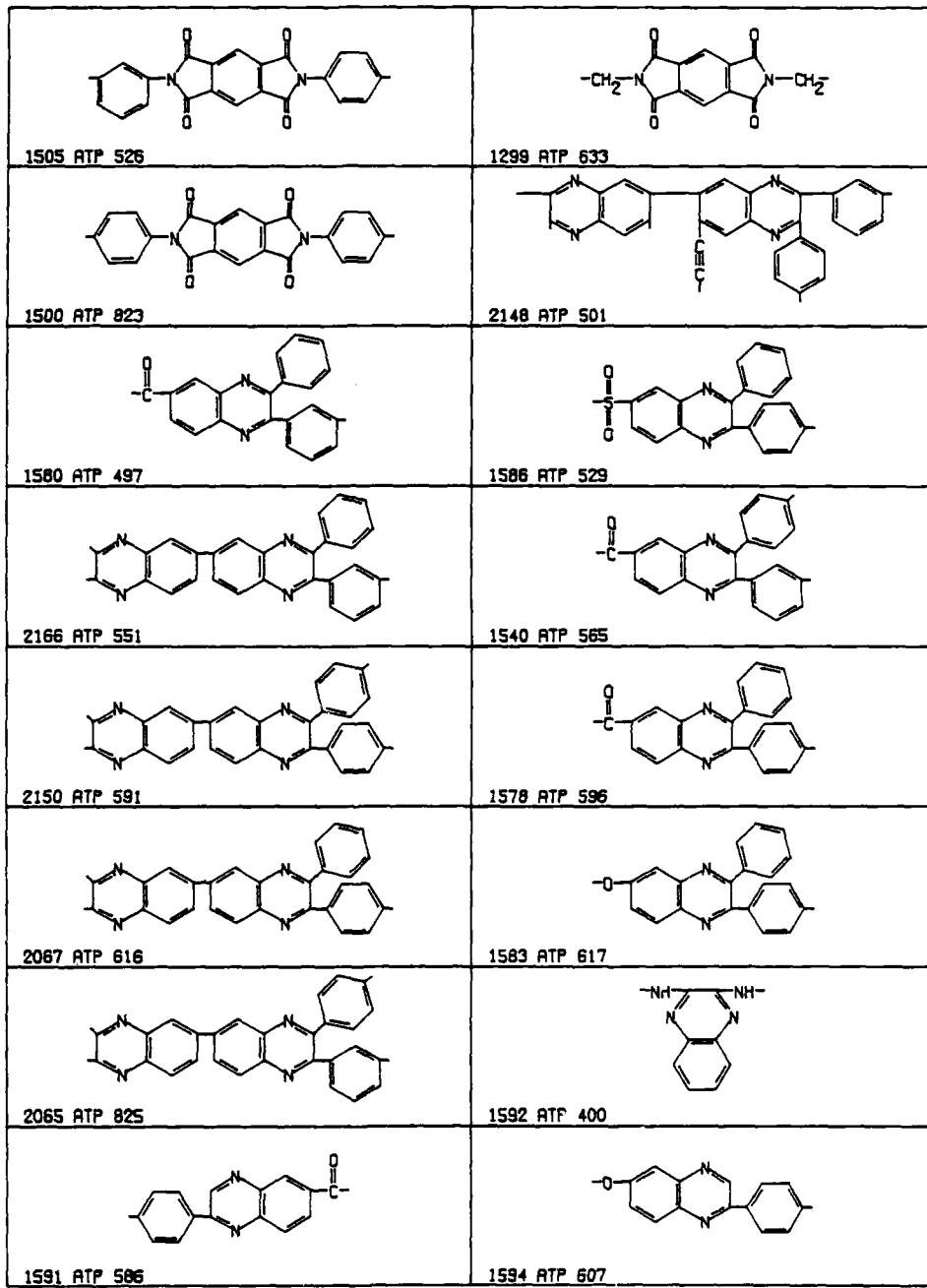
**GROUPS IN NUMERICAL ORDER OF ATP
WITHIN HIERARCHICAL ORDER OF MAIN SINGLE-GROUP**

	
1180 ATP 719	791 ATP 359
	
1185 ATP 428	1190 ATP 458
	
2080 ATP 693	2139 ATP 1043
	
1103 ATP 580	1201 ATP 583
	
1215 ATP 350	1211 ATP 360
	
1218 ATP 417	1205 ATP 452
	
2143 ATP 548	2144 ATP 787
	
1226 ATP 502	1238 ATP 409

TR 88044

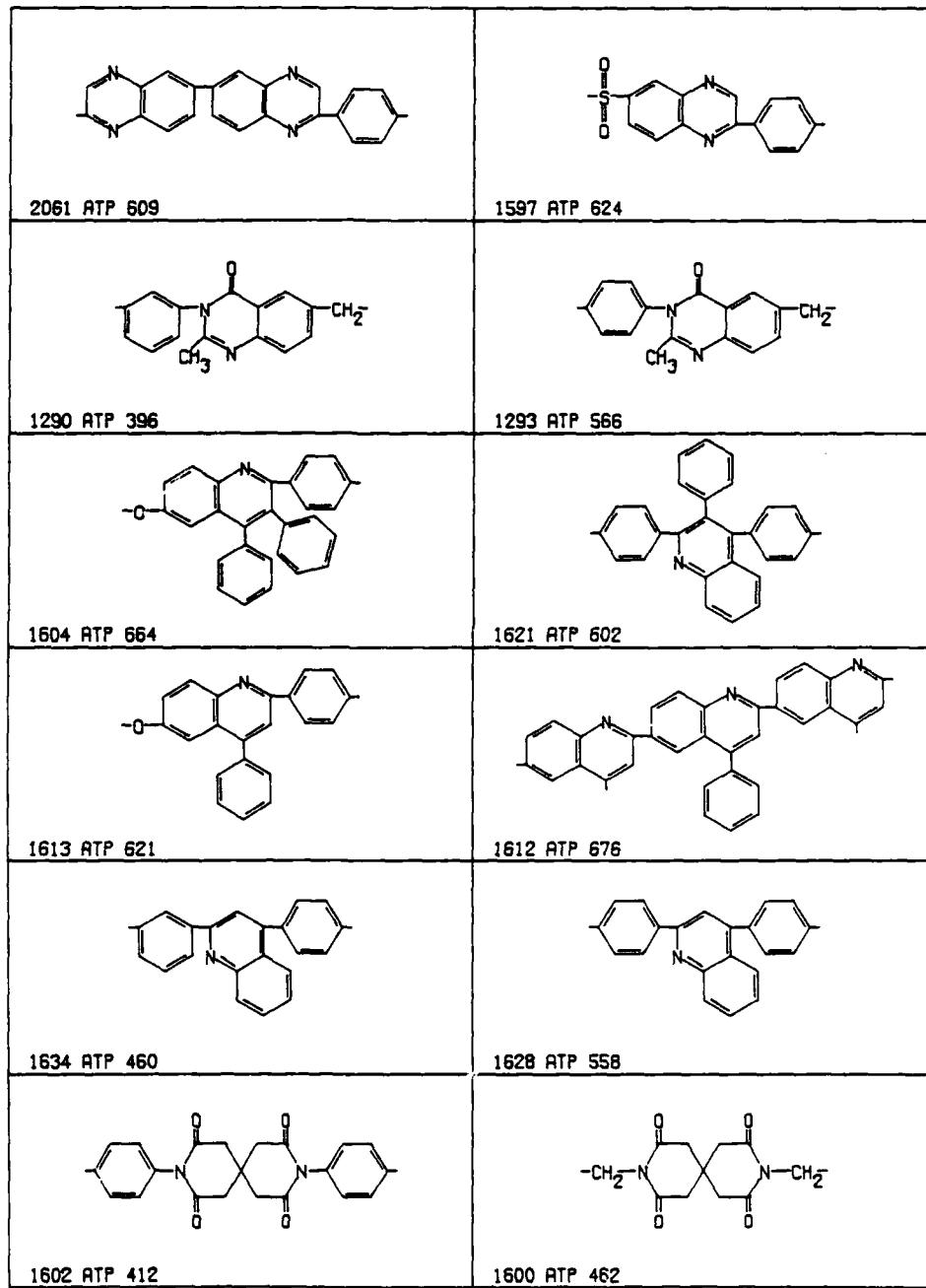


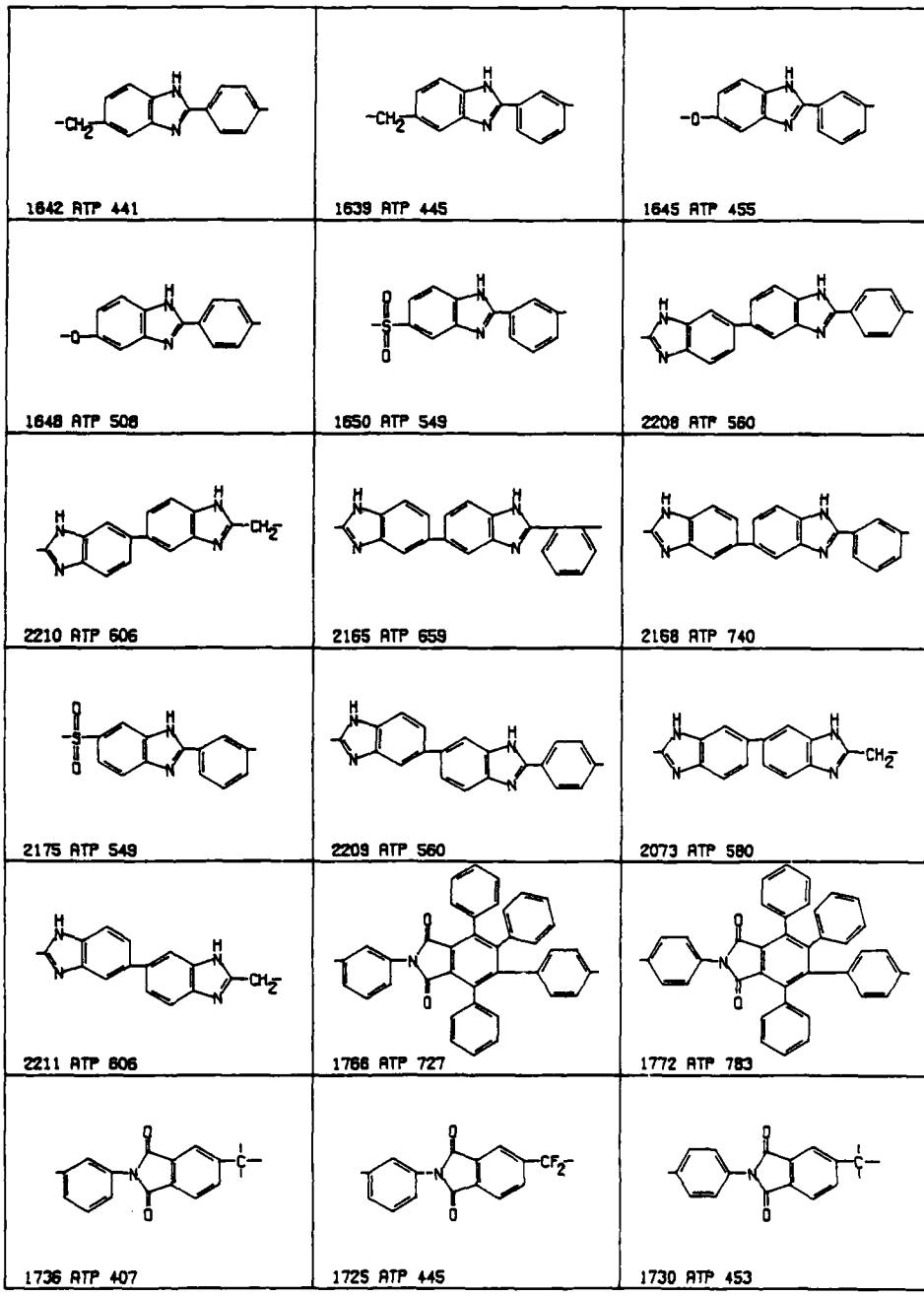
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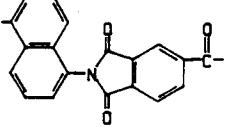
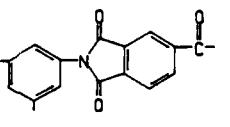
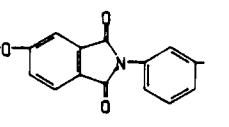
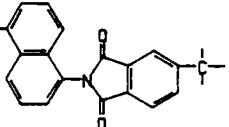
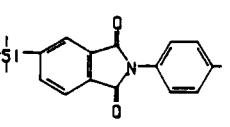
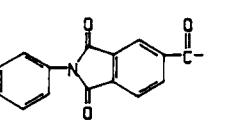
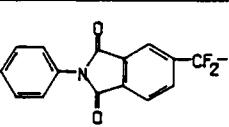
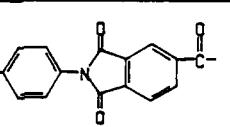
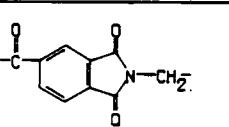
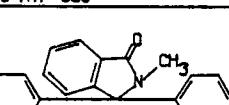
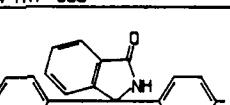
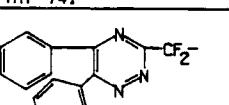
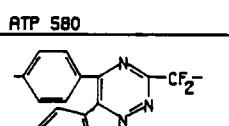
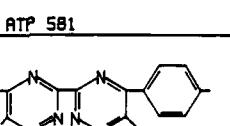
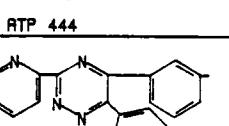
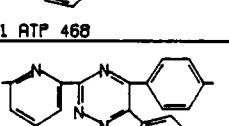
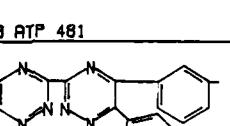
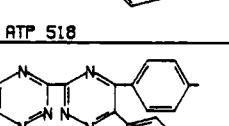
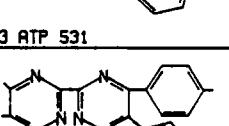
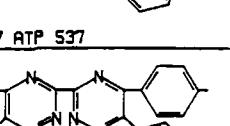
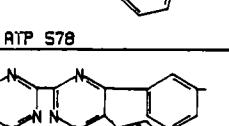
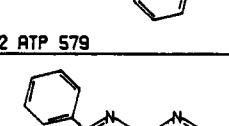
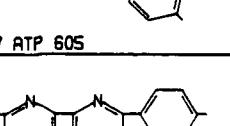
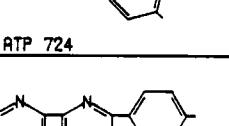
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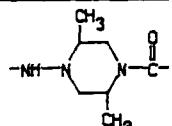
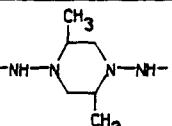
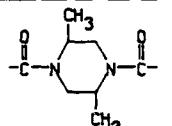
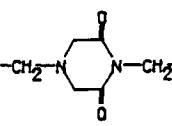
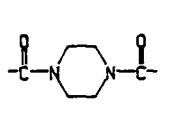
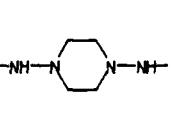
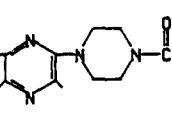
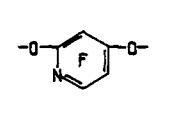
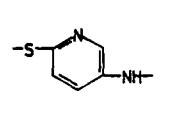
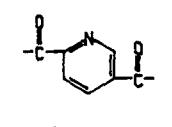
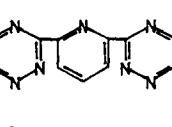
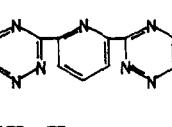
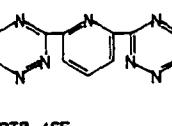
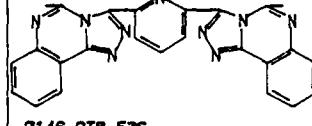
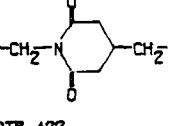
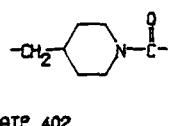
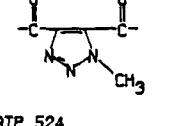
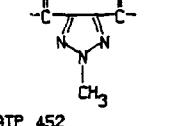
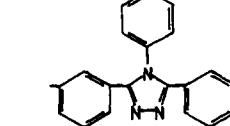
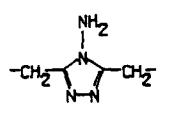
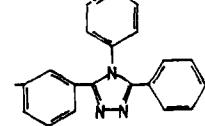
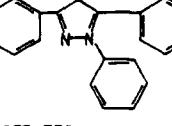
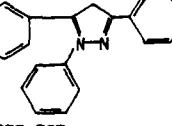
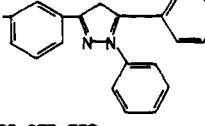
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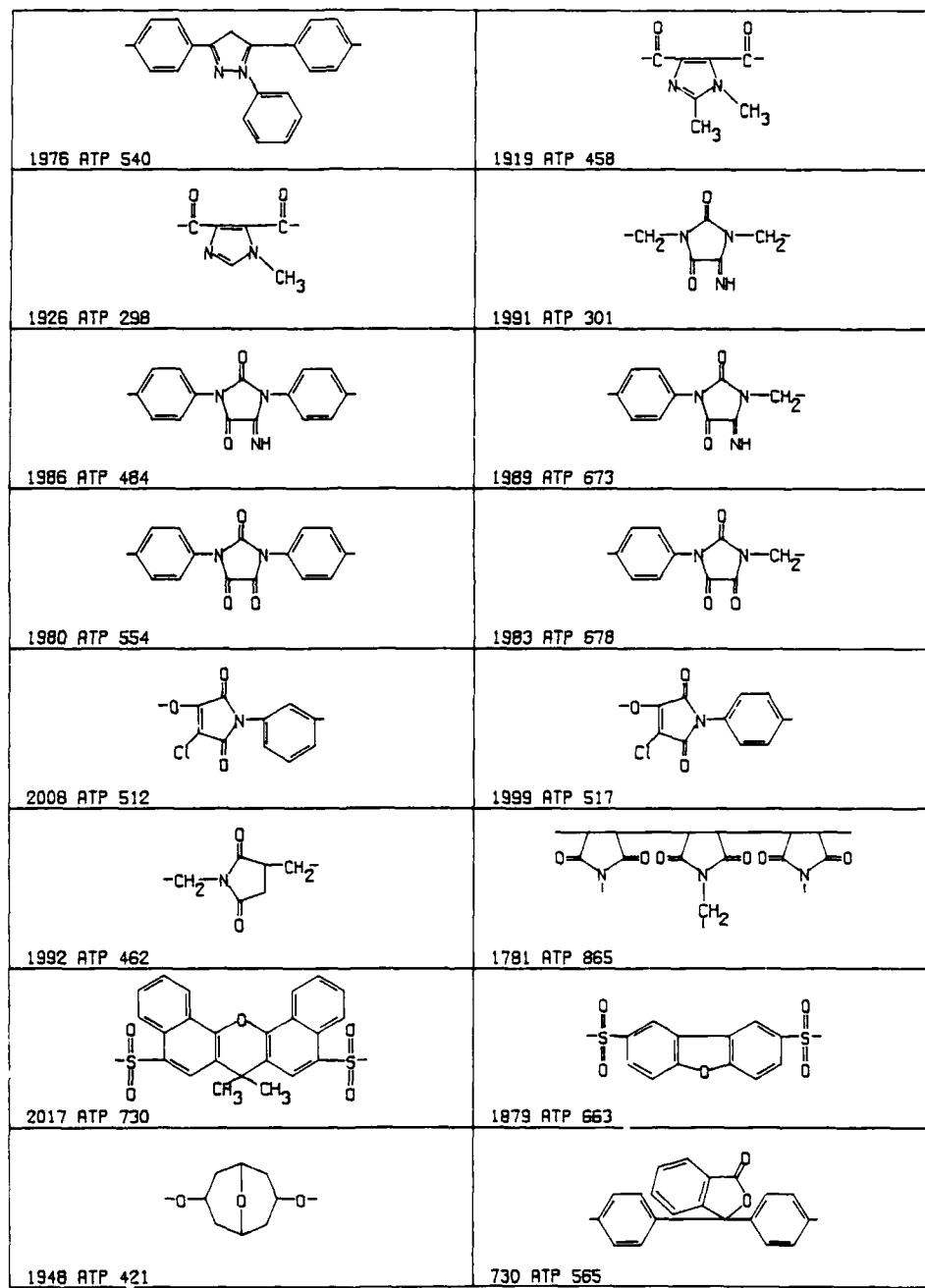
TR 88044

1871 RTP 457	594 RTP 277	595 RTP 305	1812 RTP 371
528 RTP 372	711 RTP 392	725 RTP 393	724 RTP 403
1683 RTP 475	1859 RTP 495	1845 RTP 559	1803 RTP 585
1700 RTP 600	1661 RTP 665	1800 RTP 714	1695 RTP 441
1857 RTP 450	1913 RTP 391	1915 RTP 481	1873 RTP 684
1094 RTP 503	1251 RTP 506	1956 RTP 356	1258 RTP 513

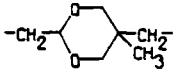
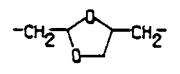
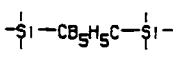
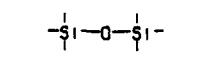
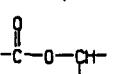
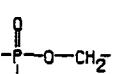
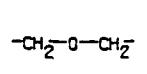
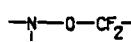
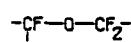
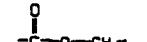
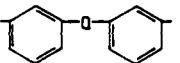
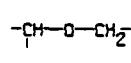
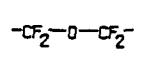
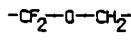
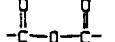
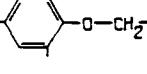
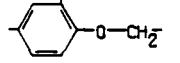
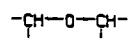
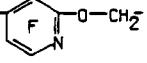
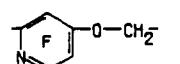
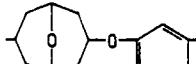
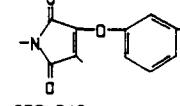
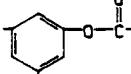
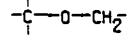
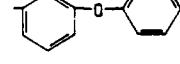
TR 890884

 1936 ATP 516	 1938 ATP 557	 1916 ATP 565
 1942 ATP 300	 438 ATP 425	 1953 ATP 426
 1250 ATP 472	 144 ATP 325	 1962 ATP 69
 1958 ATP 404	 2200 ATP 428	 2174 ATP 457
 2199 ATP 465	 2146 ATP 536	 1956 ATP 422
 1255 ATP 402	 1928 ATP 524	 1930 ATP 452
 1970 ATP 168	 1967 ATP 444	 1122 ATP 580
 1973 ATP 520	 1977 ATP 527	 1978 ATP 533

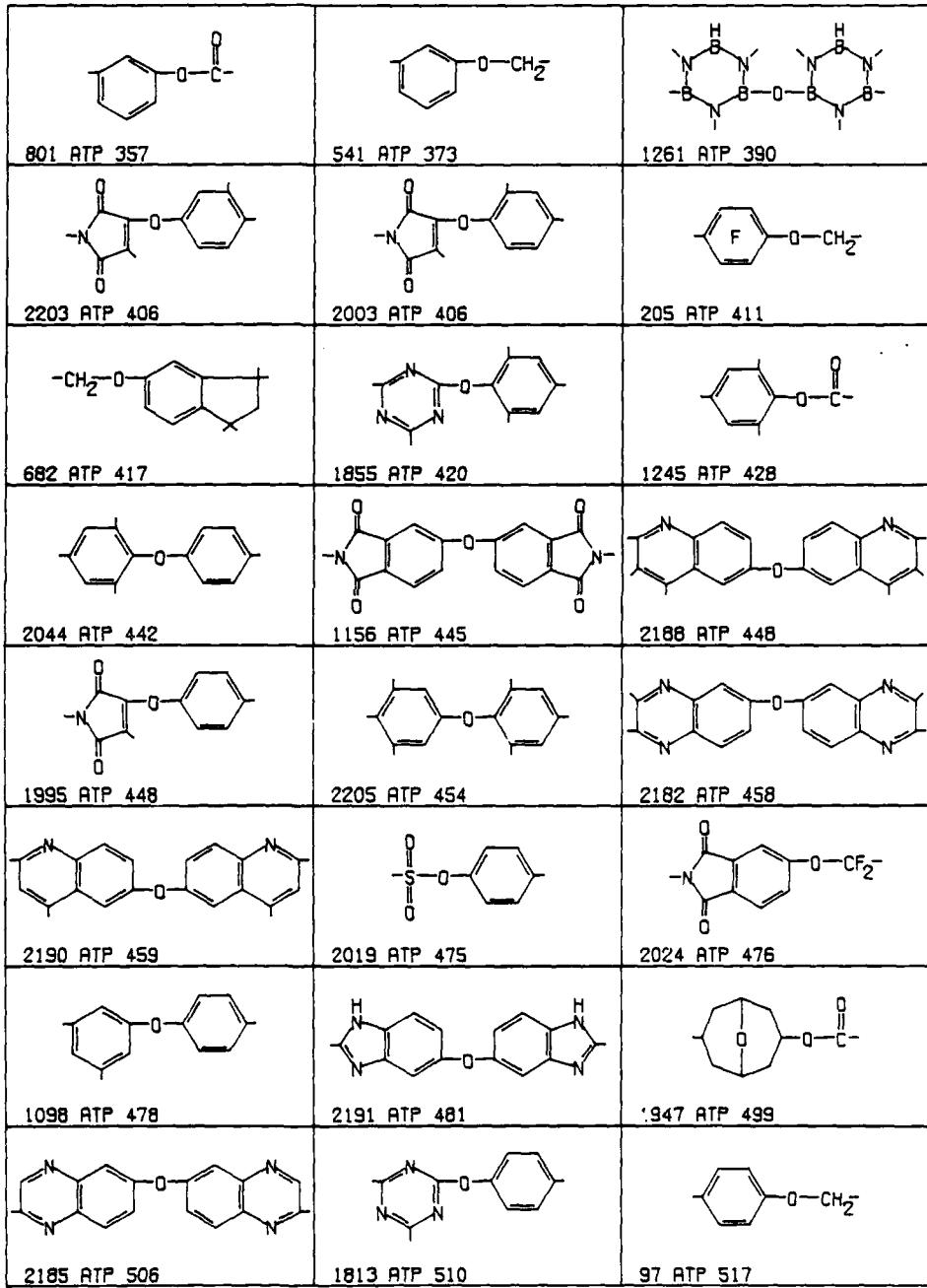
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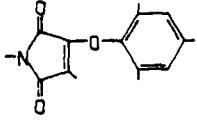
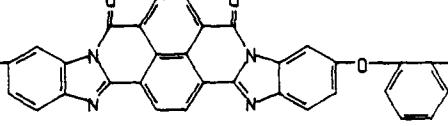
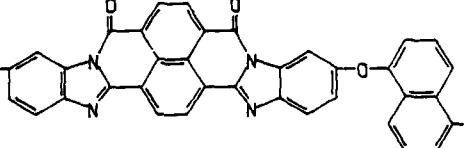
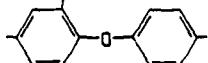
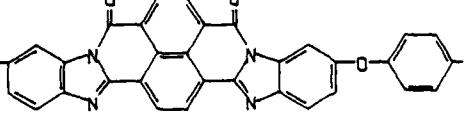
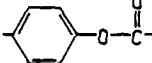
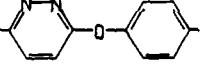
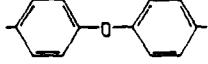
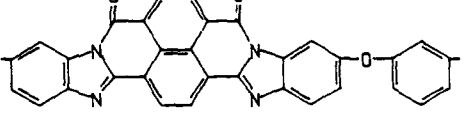
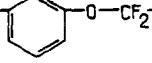
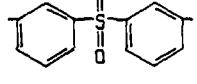
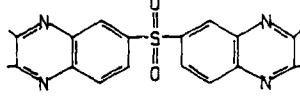
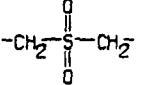
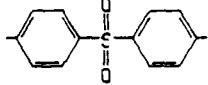


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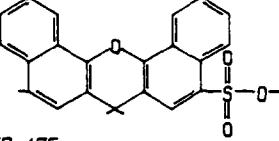
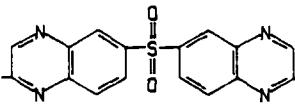
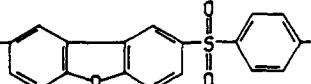
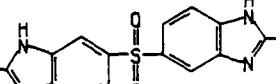
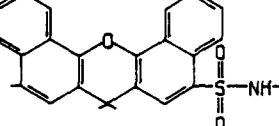
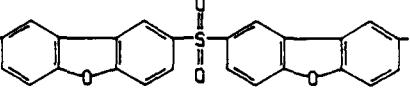
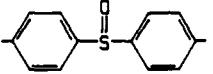
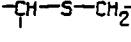
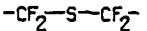
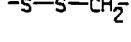
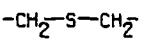
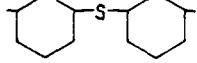
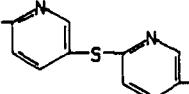
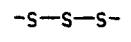
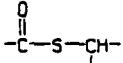
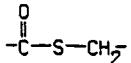
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 2015 RTP 402	 675 RTP 355	 874 RTP -52
 1000 RTP 58	 975 RTP 132	 99 RTP 174
 982 RTP 177	 433 RTP 177	 103 RTP 193
 454 RTP 239	 707 RTP 244	 452 RTP 246
 159 RTP 248	 90 RTP 254	 1400 RTP 258
 1301 RTP 267	 930 RTP 309	 816 RTP 325
 141 RTP 325	 2016 RTP 343	 2011 RTP 346
 1008 RTP 346	 877 RTP 352	 1738 RTP 355

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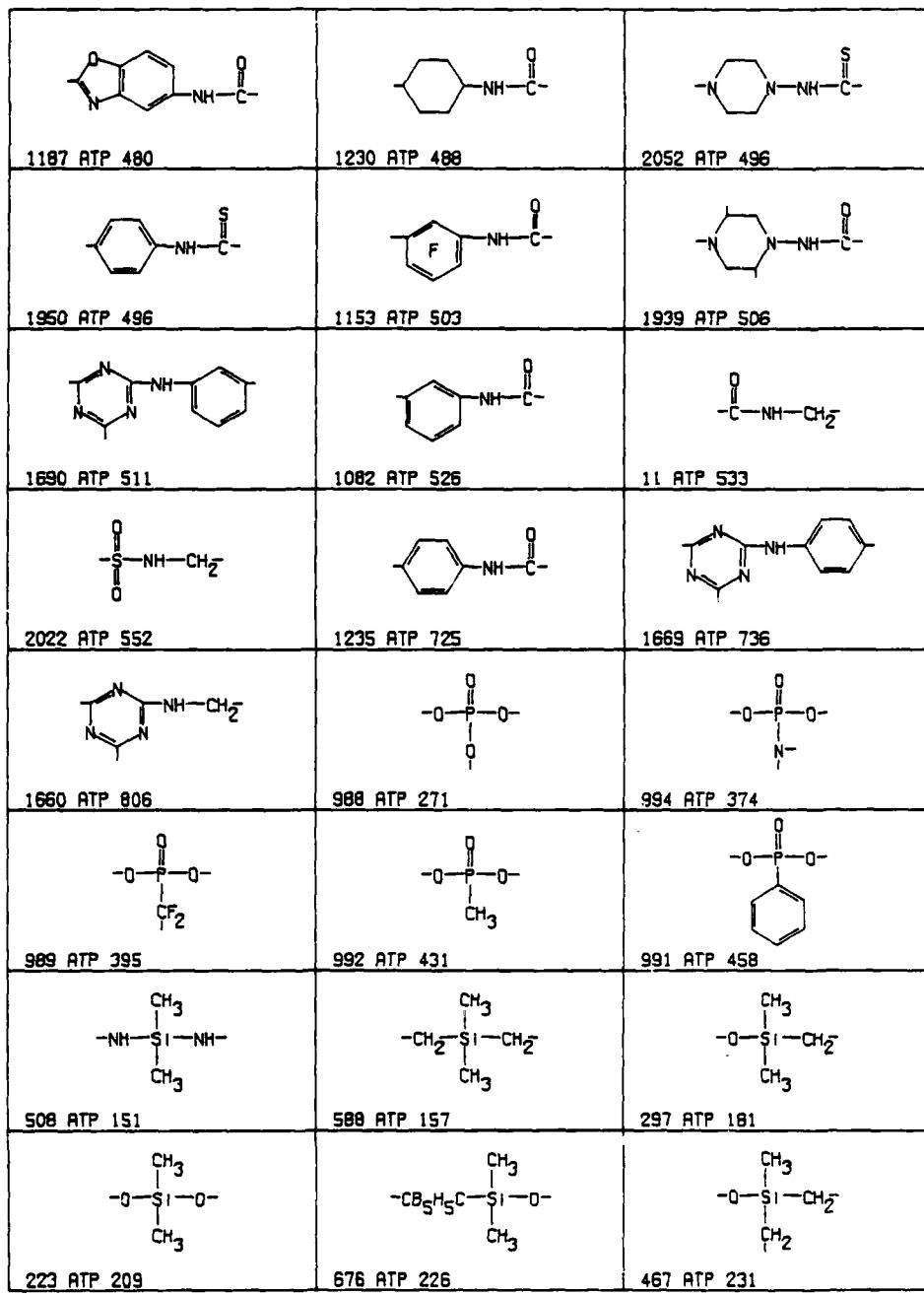
	
2202 ATP 528	1265 ATP 541
	
1267 ATP 549	2043 ATP 561
	
1270 ATP 579	109 ATP 599
	
1093 ATP 600	100 ATP 600
	
1269 ATP 620	1726 ATP 684
	
1764 ATP 280	2183 ATP 436
	
2047 ATP 446	667 ATP 460

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2018 ATP 475	2186 ATP 514
	
2049 ATP 538	2176 ATP 549
	
2021 ATP 552	1878 ATP 597
	
1108 ATP 435	546 ATP 115
	
643 ATP 131	538 ATP 165
	
295 ATP 210	578 ATP 214
	
2201 ATP 237	545 ATP 246
	
1909 ATP 320	424 ATP 412

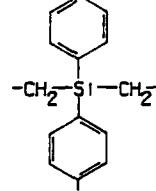
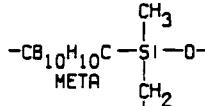
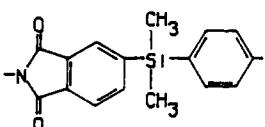
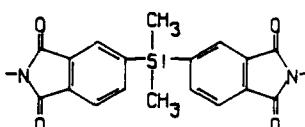
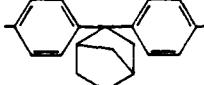
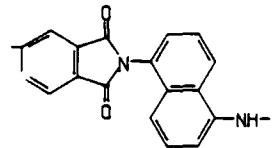
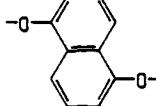
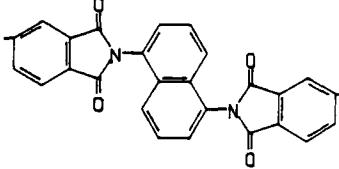
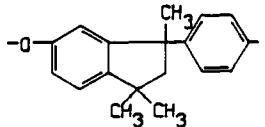
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637 RTP 205	796 RTP 209	824 RTP 259	822 RTP 352
644 RTP 378	770 RTP 169	1110 RTP 438	981 RTP 237
33 RTP 284	706 RTP 301	699 RTP 311	1240 RTP 347
610 RTP 350	1242 RTP 387	1134 RTP 431	1858 RTP 584
519 RTP 0	561 RTP 52	1963 RTP 69	602 RTP 321
1955 RTP 357	1593 RTP 395	1239 RTP 414	1937 RTP 442
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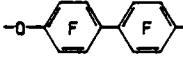
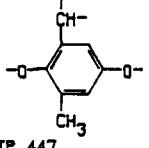
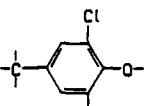
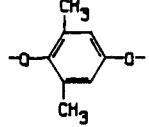
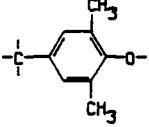
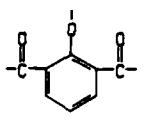
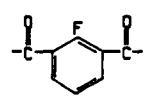
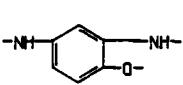
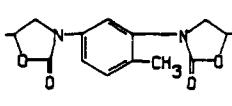
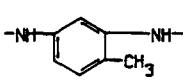
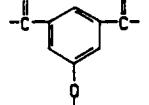
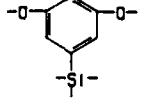
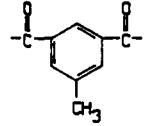
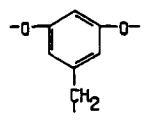
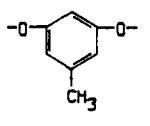
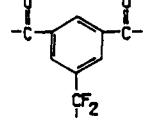
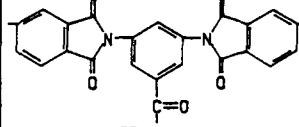
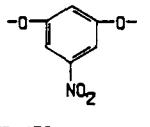
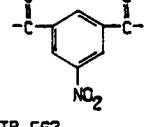
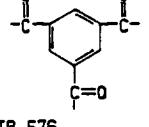
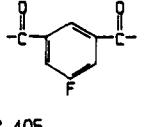
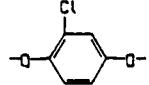
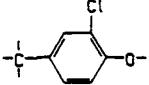
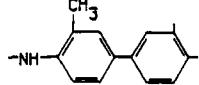
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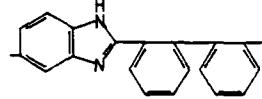
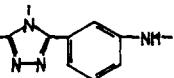
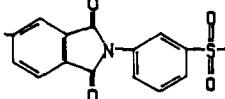
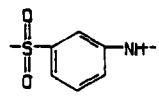
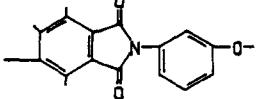
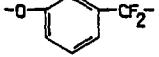
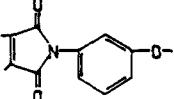
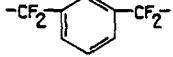
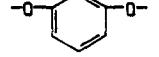
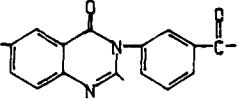
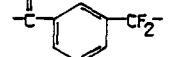
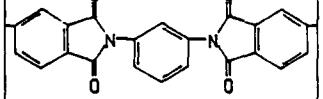
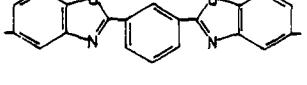
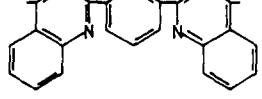
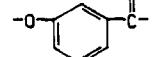
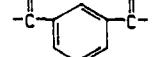
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 266 ATP 259	 710 ATP 265	 25 ATP 271
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 1143 ATP 327 META	 521 ATP 333	 1723 ATP 341
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 2014 ATP 386 PARA	 1152 ATP 389	 226 ATP 404

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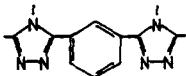
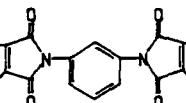
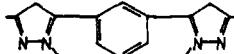
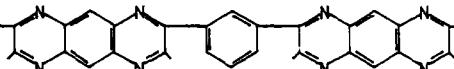
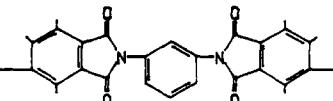
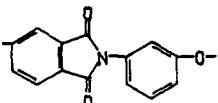
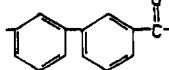
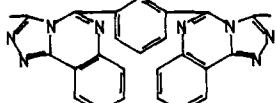
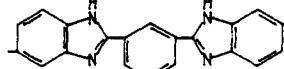
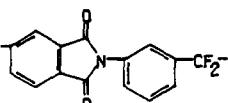
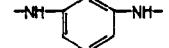
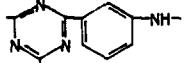
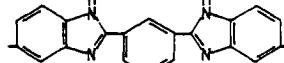
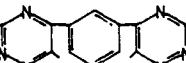
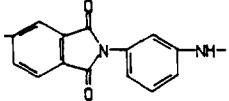
	
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461 RTP 383	1161 RTP 454

 207 RTP 411	 2115 RTP 447	 970 RTP 447
 2117 RTP 490	 1096 RTP 516	 490 RTP 443
 125 RTP 416	 574 RTP 207	 2179 RTP 350
 563 RTP 449	 483 RTP 293	 905 RTP 345
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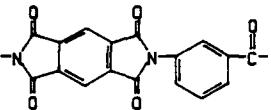
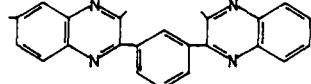
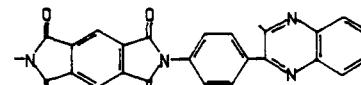
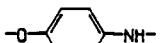
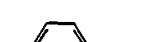
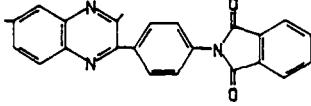
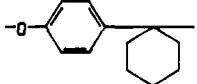
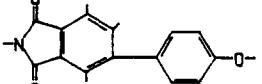
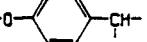
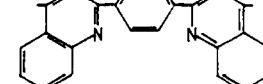
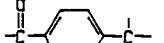
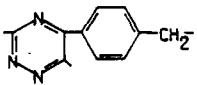
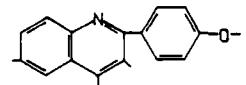
TR 88044

		
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1770 RTP 307	44 RTP 308	127 RTP 333
		
800 RTP 342	2113 RTP 346	157 RTP 377
		
1071 RTP 400	2167 RTP 401	794 RTP 401
		
2197 RTP 406	1151 RTP 416	2169 RTP 432
		
2161 RTP 433	95 RTP 433	243 RTP 444

TR 88044

	
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2137 RTP 462	2086 RTP 464
	
2084 RTP 466	1272 RTP 493
	
1200 RTP 494	2078 RTP 495
	
1727 RTP 518	799 RTP 531
	
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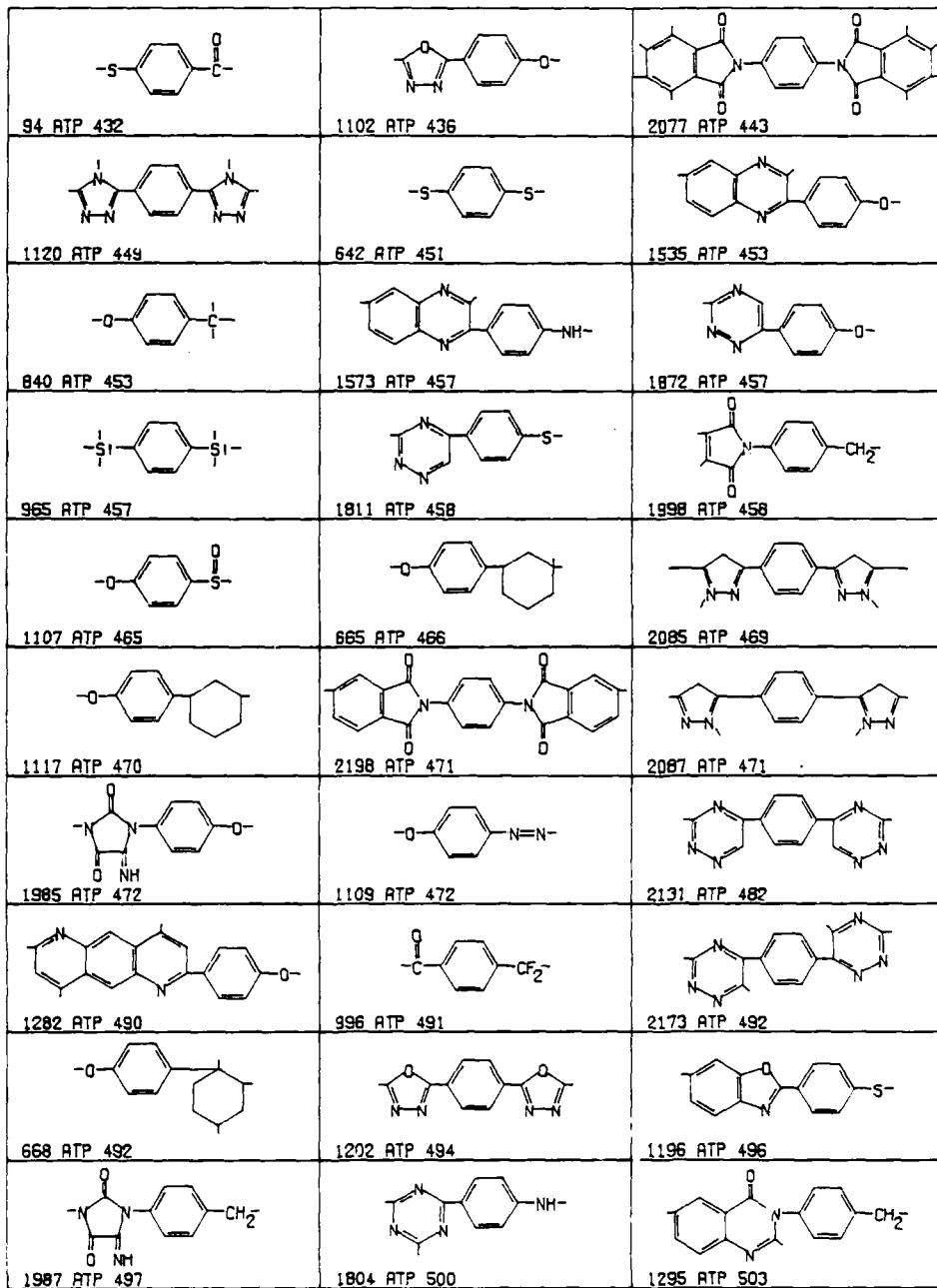
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-O-  -	-O-  -
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651 RTP 234	2184 RTP 237
-O-  -	-N-  -
129 RTP 287	1774 RTP 291
-O-  -	-  -
115 RTP 291	1531 RTP 297
-S-  -	-  -
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TR 88044

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<chem>c1ccc2c(c1)c(=O)n(-c3ccccc3)[Si-]</chem> 1724 RTP 363	<chem>[O-]c1ccccc1N[Si-]</chem> 1762 RTP 376	<chem>[O-]c1ccccc1[Si-]</chem> 24 RTP 386
<chem>c1ccc2c(c1)nc(-c3ccccc3)[O-]c2</chem> 1629 RTP 388	<chem>c1ccc2c(c1)nc(-c3ccccc3)[O-]c2</chem> 1297 RTP 392	<chem>c1ccc2c(c1)c(=O)n(-c3ccccc3)[O-]c2</chem> 1698 RTP 392
<chem>-C(=O)-C6H4-CH2-</chem> 93 RTP 397	<chem>c1ccc2c(c1)c(=O)n(-c3ccccc3)Nc2</chem> 1292 RTP 401	<chem>-N1CC=CC=C1-</chem> 1243 RTP 401
<chem>c1ccc2c(c1)c(=O)n(-c3ccccc3)S-</chem> 1740 RTP 405	<chem>c1ccc2c(c1)c(=O)n(-c3ccccc3)[O-]c2</chem> 2010 RTP 409	<chem>c1ccc2c(c1)c(=O)n(-c3ccccc3)[O-]c2</chem> 1775 RTP 410
<chem>-O-C6H4-C6H4-</chem> 1113 RTP 414	<chem>c1c[nH]c2c(c1)sc(-c3ccccc3)[Si-]2-</chem> 1844 RTP 417	<chem>c1ccc2c(c1)C(Oc3ccccc3)C2-</chem> 959 RTP 417
<chem>c1ccc2c(c1)nc(-c3ccccc3)[O-]c2</chem> 1530 RTP 419	<chem>c1ccc2c(c1)C(=O)C3C(Nc4ccccc4)C(=O)C3Nc2-</chem> 1603 RTP 420	<chem>c1ccc2c(c1)c(=O)n(-c3ccccc3)CH2-</chem> 1777 RTP 420
<chem>c1ccc2c(c1)c(=O)n(-c3ccccc3)CH2-</chem> 1697 RTP 420	<chem>c1ccc2c(c1)ccc3c(c2)nc4ccccc4n3</chem> 2157 RTP 422	<chem>c1c[nH]c2c(c1)sc(-c3ccccc3)[O-]c2</chem> 1824 RTP 425
<chem>Oc1ccccc1</chem> 660 RTP 427	<chem>c1ccc2c(c1)ccc3c(c2)nc4ccccc4n3</chem> 2160 RTP 430	<chem>c1c[nH]c2c(c1)sc(-c3ccccc3)[O-]c2</chem> 1809 RTP 430

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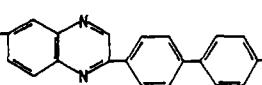
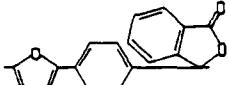
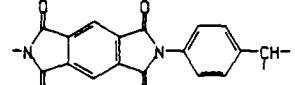
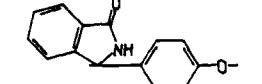
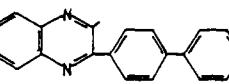
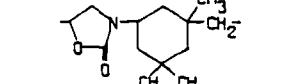
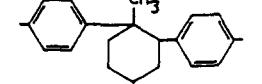
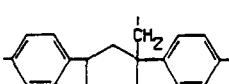
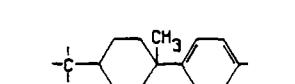
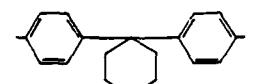
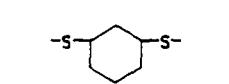
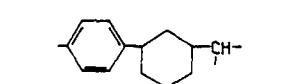
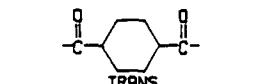
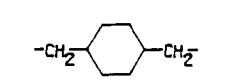
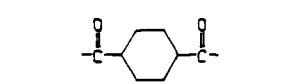
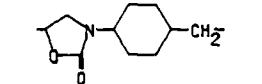
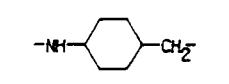
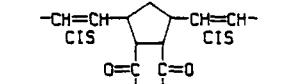
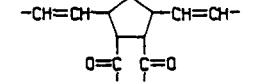
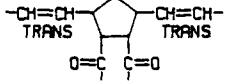
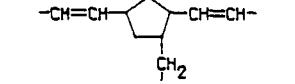
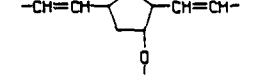
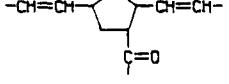
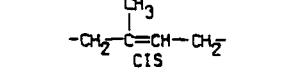


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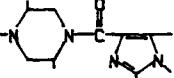
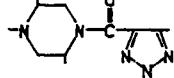
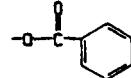
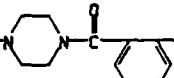
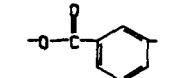
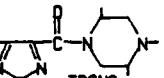
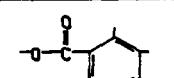
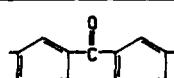
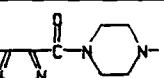
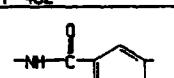
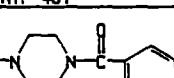
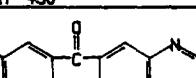
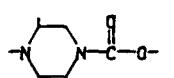
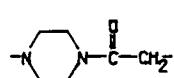
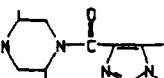
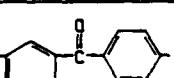
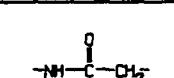
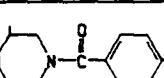
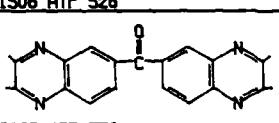
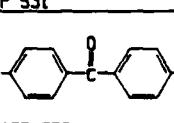
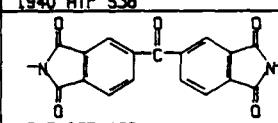
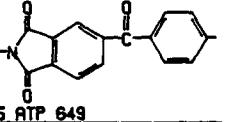
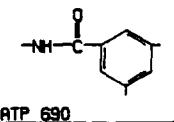
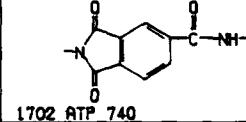
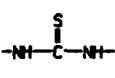
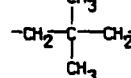
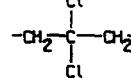
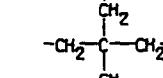
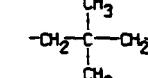
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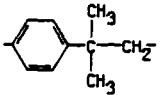
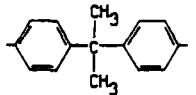
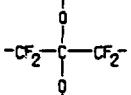
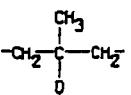
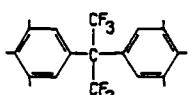
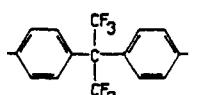
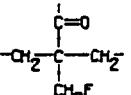
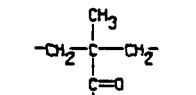
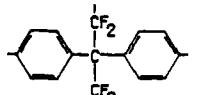
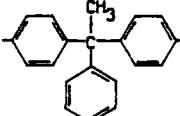
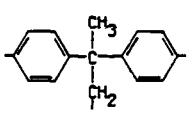
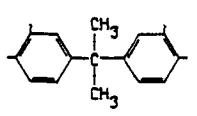
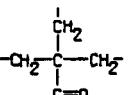
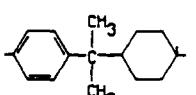
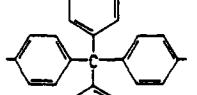
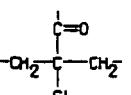
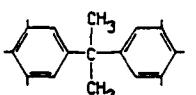
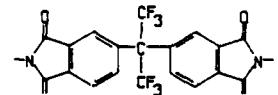
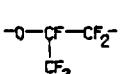
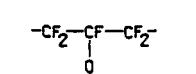
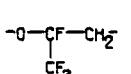
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 445 RTP 202	 177 RTP 218	 178 RTP 232	 3 RTP 238
 596 RTP 257	 1920 RTP 265	 1925 RTP 298	 1911 RTP 320
 1004 RTP 329	 110 RTP 347	 1954 RTP 357	 1710 RTP 360
 1917 RTP 366	 599 RTP 368	 590 RTP 383	 1957 RTP 385
 1905 RTP 394	 1228 RTP 399	 87 RTP 401	 1257 RTP 402
 1959 RTP 404	 117 RTP 405	 104 RTP 405	 556 RTP 412
 126 RTP 426	 1244 RTP 428	 1227 RTP 428	 544 RTP 439

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 646 ATP 311	 89 ATP 323	 50 ATP 339
 1074 ATP 350	 2145 ATP 370	 827 ATP 377
 788 ATP 387	 148 ATP 389	 171 ATP 404
 654 ATP 409	 839 ATP 414	 2132 ATP 431
 807 ATP 458	 657 ATP 468	 1114 ATP 475
 330 ATP 492	 2089 ATP 517	 2074 ATP 713
 39 ATP 214	 55 ATP 254	 2055 ATP 255

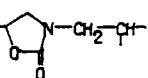
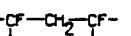
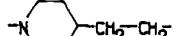
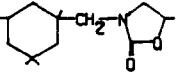
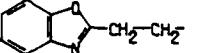
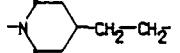
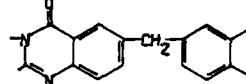
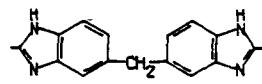
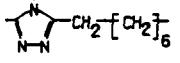
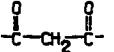
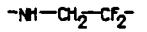
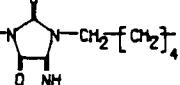
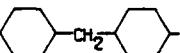
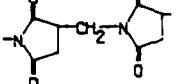
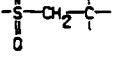
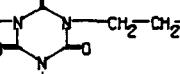
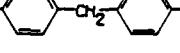
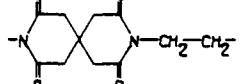
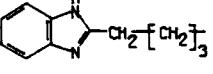
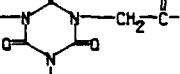
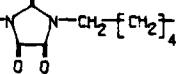
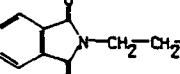
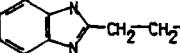
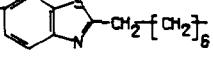
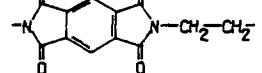
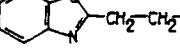
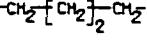
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84 RTP 268	529 RTP 289	132 RTP 299	169 RTP 345
<chem>-CF2-C(F)(Cl)CF2-</chem>	<chem>-CF2-C(F)(C(F)(F)Cl)CF2-</chem>	<chem>-CH2-C(F)(C(F)(F)Cl)CH2-</chem>	<chem>-CF2-C(F)(C(F)(F)Cl)CF2-</chem>
137 RTP 381	792 RTP 465	817 RTP 468	195 RTP 519
<chem>-CF2-CF2-CF2-</chem>	<chem>-N(CF2-CF2)-</chem>	<chem>-O-CF2-CF2-</chem>	<chem>-S-CF2-S-</chem>
165 RTP 123	1076 RTP 177	26 RTP 184	751 RTP 185
<chem>-CH2-CF2-CH2-</chem>	<chem>N1C=NC2=C1C(F)(F)OC(F)(F)C(F)(F)C2</chem>	<chem>O=C(C(F)(F)Cl)CF2-</chem>	<chem>N1C=NC2=C1C(F)(F)OC(F)(F)C(F)(F)C2</chem>
494 RTP 228	525 RTP 252	597 RTP 257	592 RTP 281
<chem>N1C=NC2=C1C(F)(F)S2-</chem>	<chem>-CF2-CF2-CH2-</chem>	<chem>-CH-C(F)(F)C(F)C(F)O</chem>	<chem>-O-CF2-C(F)C(F)O</chem>
526 RTP 298	10 RTP 300	135 RTP 309	36 RTP 310
<chem>-C(F)C(F)CF-</chem>	<chem>-O-CF2-CH2-</chem>	<chem>-C(F)C(F)C(F)C(F)O</chem>	<chem>c1ccccc1-CF2-CF2-</chem>
138 RTP 329	203 RTP 331	51 RTP 339	795 RTP 358
<chem>c1cc2oc(c2)C(F)(F)CF2-</chem>	<chem>c1cc2oc(c2)C(F)(F)OC(F)(F)C(F)(F)C2</chem>	<chem>c1ccccc1-CF2-CF2-</chem>	<chem>c1cc2oc(c2)C(F)(F)OC(F)(F)C(F)(F)C2</chem>
1050 RTP 359	1111 RTP 366	997 RTP 393	1063 RTP 398
<chem>N1C=NC2=C1C(F)(F)CF2-</chem>	<chem>-N1C(=O)c2ccccc2C(F)(F)CF2-</chem>	<chem>-CF2-[CF2]2-CF2-</chem>	<chem>-CF2-[CF2]3-CF2-</chem>
1849 RTP 456	1006 RTP 630	1402 RTP 213	1403 RTP 201
<chem>-CF2-[CF2]4-CF2-</chem>	<chem>-CF2-[CF2]5-CF2-</chem>	<chem>-CF2-[CF2]6-CF2-</chem>	<chem>-CF2-[CF2]8-CF2-</chem>
1404 RTP 240	1405 RTP 304 SYNDIOTACTIC <chem>-CH2-C(F)(CH2)CH2-</chem>	1406 RTP 232	1408 RTP 295
<chem>-CF2-[CF2]n-CF2-</chem>	531 RTP 216	<chem>-O-CH2-CH2-</chem>	<chem>-CH=CH-CH(Cis)-CH2-</chem>
1421 RTP 400		572 RTP 67	372 RTP 171

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<chem>-CH2-C(=O)CH2-</chem> 459 RTP 185	<chem>-O-CH(CH3)CH2-</chem> 435 RTP 195	<chem>-S-CH(CH2)CH2-</chem> 547 RTP 197	<chem>-O-CH(O-CH3)-</chem> 455 RTP 213	<chem>-S-CH(C(=O)CH3)-</chem> 1910 RTP 235
<chem>-S-CH(CH3)CH2-</chem> 184 RTP 240	<chem>-CH2-CH(CH2)CH2-</chem> 74 RTP 251	<chem>-CH(CH2)CH(Cl)CH2-</chem> 385 RTP 272	<chem>-CH2-CH(CH3)CH2-</chem> 431 RTP 280	<chem>-CH2-CH(CH2)CH2-</chem> 403 RTP 289
<chem>-O-CH(CH2)C(F)(F)2-</chem> 436 RTP 293	<chem>-CH2-CH(C(=O)F)CH2-</chem> 56 RTP 299	<chem>-CF2-CH(C(=O)F)CH2-</chem> 136 RTP 309	<chem>-C(=O)CH(C(=O)CH2)C(=O)-</chem> 176 RTP 324	<chem>-CH2-CH(CH2)S-</chem> 1047 RTP 335
<chem>-CH2-CH(C(F)(F)3)CH2-</chem> 715 RTP 336	<chem>-CH2-CH(CH3)C6H4CH2-</chem> 649 RTP 342	<chem>-CH2-CH(C6H4CH2)C6H4CH2-</chem> 712 RTP 352	<chem>-CH2-CH(CH3)C6H4CH2-</chem> 128 RTP 352	<chem>-CH2-CH(C(F)(F)3)CH2-</chem> 107 RTP 373
<chem>-C(=O)CH(C(=O)CH3)C(=O)-</chem> 784 RTP 380	<chem>-CH2-CH(C6H4)CH2-</chem> 66 RTP 387	<chem>-O-CH(CH2)C(=O)I-</chem> 973 RTP 389	<chem>-CH2-CH(OH)CH2-</chem> 503 RTP 409	<chem>-CH2-CH(C6H4)CH2-</chem> 842 RTP 417
<chem>-CH2-CH(C6H5)CH2-</chem> 856 RTP 417	<chem>-O-CH(C6H5)CH2-</chem> 708 RTP 421	<chem>-CH2-CH(C6H4F)CH2-</chem> 1148 RTP 421	<chem>-CH2-CH(C6H4F)CH2-</chem> 1149 RTP 424	<chem>-CH2-CH(C6H4F)CH2-</chem> 85 RTP 437
<chem>-CH2-CH(C6H5F)CH2-</chem> 1150 RTP 437	<chem>-CH2-CH(C6H4F)CH2-</chem> 172 RTP 446	<chem>-CH2-CH(C6H4N)CH2-</chem> 756 RTP 447	<chem>-CH2-CH(C6H5)CH2-</chem> 860 RTP 458	<chem>-CH2-CH(C6H4CH3)C1CCCCC1-</chem> 1115 RTP 535
<chem>-CH2-CH(C6H4CH2)CH2-</chem> 843 RTP 547	<chem>-CH2-CH(C6H5)CH2-</chem> 904 RTP 571	<chem>-CH2-CH(C6H5)CH2-</chem> 373 RTP 695	<chem>-CF(CF3)CH(CF3)CF-</chem> 134 RTP 299	<chem>-CF(CF3)CH(CF3)CF-</chem> 761 RTP 356
<chem>-CN=C(CH2)CH2CH2-</chem> CIS 122 RTP 127	<chem>-CH2-CH2-CH2-</chem> TRANS 13 RTP 133	<chem>-CH=CH-CH2-CH2-</chem> TRANS 123 RTP 149	<chem>-C=C(CH2)CH2-CH2-</chem> TRANS 849 RTP 166	<chem>-O-CH2-CH-</chem> 645 RTP 170

$-O-CH_2-CF_2-$	$-CH-CH_2-CH_2-$	$-C=CH-CH_2-CH_2-$ CIS	$-O-CH_2-O-$	$-C(=O)-CH_2-CH-$
797 RTP 183	630 RTP 183	891 RTP 203	426 RTP 213	291 RTP 227
$-CH-CH_2-CH-$	$-S-CH_2-S-$	$-O-CH_2-CH_2-$	$-O-CH_2-C-$	$-S-CH_2-SI-$
833 RTP 230	543 RTP 231	98 RTP 234	846 RTP 241	589 RTP 241
$-S-CH_2-C-$	$-CF_2-CH_2-CF_2-$	$-N-CH_2-CH_2-$	$C(=O)-CH_2-CH_2-$	$-S-CH_2-CH_2-$
555 RTP 242	493 RTP 244	1106 RTP 253	14 RTP 256	102 RTP 275
$-CH=CH-CH_2-CH-$ CIS	$-NH-CH_2-$	$-SI-CH_2-CH_2-$	$-O-CH_2-$	$-S-CH_2-CH-$
375 RTP 288	1232 RTP 293	468 RTP 296	43 RTP 297	551 RTP 297
	$-S-CH_2-C(=O)-$	$-C-CH_2-C-$	SYNDIOTACTIC $-CH-CH_2-CH-$	$-O-CH_2-$
1941 RTP 300	593 RTP 306	809 RTP 306	535 RTP 310	46 RTP 313
$-CH_2-CH_2-\text{cyclic structure}$	$-O-CH_2-CF-$	$-SI-CH_2-C-$	$-CH_2-O-$	$[CH_2]_5-CH_2-$
656 RTP 327	2054 RTP 330	1015 RTP 331	674 RTP 340	632 RTP 340
$-CH_2-CH_2-$	$-N-CH_2-$	$-O-CH_2-$	$-O-CH_2-$	$-CH_2-CH_2-$
540 RTP 341	1876 RTP 343	669 RTP 346	1900 RTP 355	871 RTP 356
$-CH_2-CH_2-N-$	$-N-CH_2-$	$-NH-CH_2-$	$-C-CH_2-CH-$	$-O-CH_2-$
1213 RTP 359	1944 RTP 362	523 RTP 362	627 RTP 363	1204 RTP 364
$-S-CH_2-$	$-N-$	$-CF_2-CH_2-CH_2-$	$-NH-CH_2-CH_2-$	$-C-CH_2-CH_2-$
559 RTP 366	1993 RTP 367	469 RTP 367	12 RTP 374	830 RTP 389

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$-\text{CH}_2-\text{[CH}_2\text{]}_3-\text{CH}_2-$	$-\text{CH}_2-\text{[CH}_2\text{]}_4-\text{CH}_2-$	$-\text{CH}_2-\text{[CH}_2\text{]}_5-\text{CH}_2-$	$-\text{CH}_2-\text{[CH}_2\text{]}_6-\text{CH}_2-$	$-\text{CH}_2-\text{[CH}_2\text{]}_7-\text{CH}_2-$
1303 RTP 204	1304 RTP 215	1305 RTP 201	1306 RTP 303	1307 RTP 208
$-\text{CH}_2-\text{[CH}_2\text{]}_8-\text{CH}_2-$	$-\text{CH}_2-\text{[CH}_2\text{]}_9-\text{CH}_2-$	$-\text{CH}_2-\text{[CH}_2\text{]}_{12}-\text{CH}_2-$	$-\text{CH}_2-\text{[CH}_2\text{]}_{14}-\text{CH}_2-$	$-\text{CH}_2-\text{[CH}_2\text{]}_n-\text{CH}_2-$
1308 RTP 226	1309 RTP 226	1312 RTP 260	1314 RTP 194	1321 RTP 155
625 RTP 70	163 RTP 126	49 RTP 140	471 RTP 189	726 RTP 191
586 RTP 207	164 RTP 213	48 RTP 224	2212 RTP 227	58 RTP 233
750 RTP 253	636 RTP 254	259 RTP 256	443 RTP 257	63 RTP 267
979 RTP 271	497 RTP 274	925 RTP 284	716 RTP 285	584 RTP 291

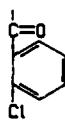
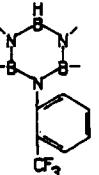
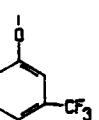
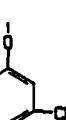
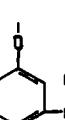
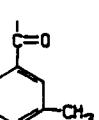
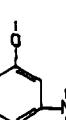
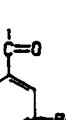
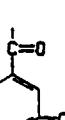
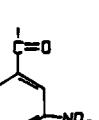
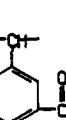
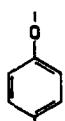
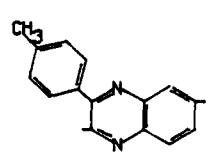
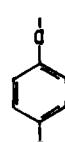
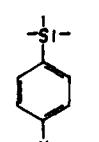
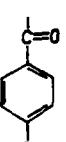
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629 RTP 352	61 RTP 354	190 RTP 362	614 RTP 363	1049 RTP 381	718 RTP 382
1033 RTP 385	1030 RTP 387	5 RTP 391	319 RTP 392	903 RTP 400	232 RTP 404
995 RTP 405	367 RTP 415	1056 RTP 423	481 RTP 443	1543 RTP 446	349 RTP 454
623 RTP 459	681 RTP 485	1174 RTP 495	189 RTP 534	6 RTP 563	781 RTP 579

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698 ATP 590	1052 ATP 323	742 ATP 225	1048 ATP 266	752 ATP 305	821 ATP 209
647 ATP 241	694 ATP 278	606 ATP 285	1070 ATP 296	1046 ATP 310	1065 ATP 367
1157 ATP 384	1692 ATP 479	400 ATP 503	1671 ATP 508	1663 ATP 606	818 ATP 153
1170 ATP 305	399 ATP 420	316 ATP 424	396 ATP 490	393 ATP 506	951 ATP 163
612 ATP 185	915 ATP 223	929 ATP 223	780 ATP 319	1057 ATP 514	746 ATP 374
1062 ATP 343	274 ATP 429	820 ATP 436	1172 ATP 511	355 ATP 442	1037 ATP 346

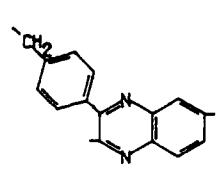
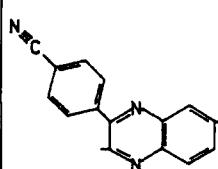
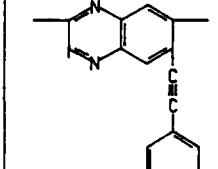
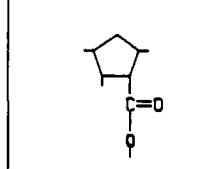
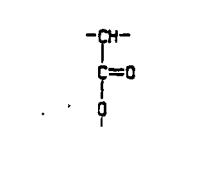
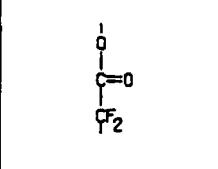
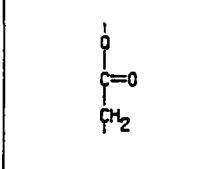
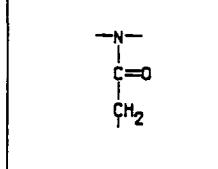
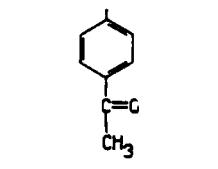
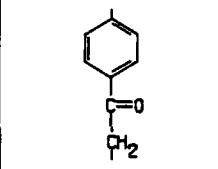
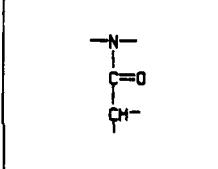
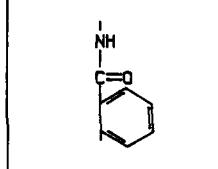
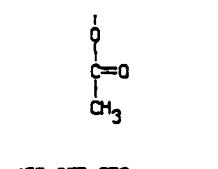
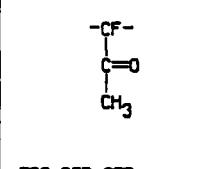
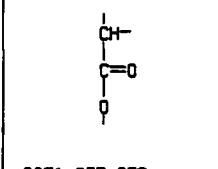
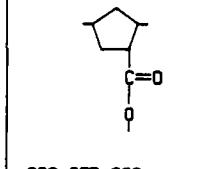
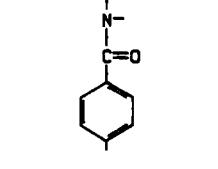
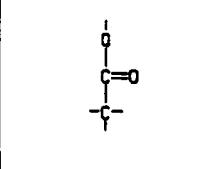
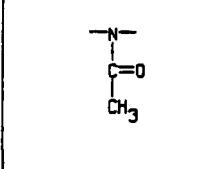
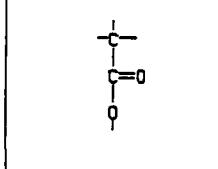
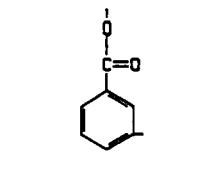
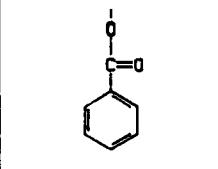
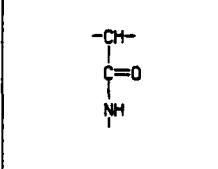
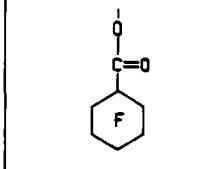
TR 880/4

			
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1041 RTP 396	1039 RTP 415	1025 RTP 494	1171 RTP 571
			
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1059 RTP 339	632 RTP 343	605 RTP 365	1035 RTP 368

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 113 RTP 407	 1023 RTP 408	 782 RTP 414	 1819 RTP 417
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 628 RTP 446	 1542 RTP 497	 1558 RTP 501	 1027 RTP 512
 1553 RTP 513	 1831 RTP 526	 1544 RTP 585	 1829 RTP 579
 1536 RTP 616	 1827 RTP 627	 1825 RTP 631	 980 RTP 651

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777 RTP 354	253 RTP 359	1142 RTP 363	990 RTP 395	173 RTP 401	185 RTP 404	114 RTP 407

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1456 RTP 219	1457 RTP 305	238 RTP 138	1241 RTP 231	237 RTP 232	290 RTP 258	1043 RTP 275
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741 RTP 54	548 RTP 90	924 RTP 115	59 RTP 129	557 RTP 138	814 RTP 147	841 RTP 158
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1364 RTP 271	1365 RTP 285	1366 RTP 311

TR 8804

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<u>No.</u>	<u>Author</u>	<u>Title, etc</u>
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Table 2

ERROR IN CALCULATED TG ASSOCIATED WITH POLYMERS AND TG RELATIONSHIPS

TABLE 2

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ERROR IN CALCULATED TG ASSOCIATED WITH POLYMERS AND TG
RELATIONSHIPS

Table 5

POLYMERS ASSOCIATED WITH A PARTICULAR ERROR IN CALCULATED TGS

TABLE 5

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POLYMERS ASSOCIATED WITH A PARTICULAR ERROR IN
CALCULATED TGS

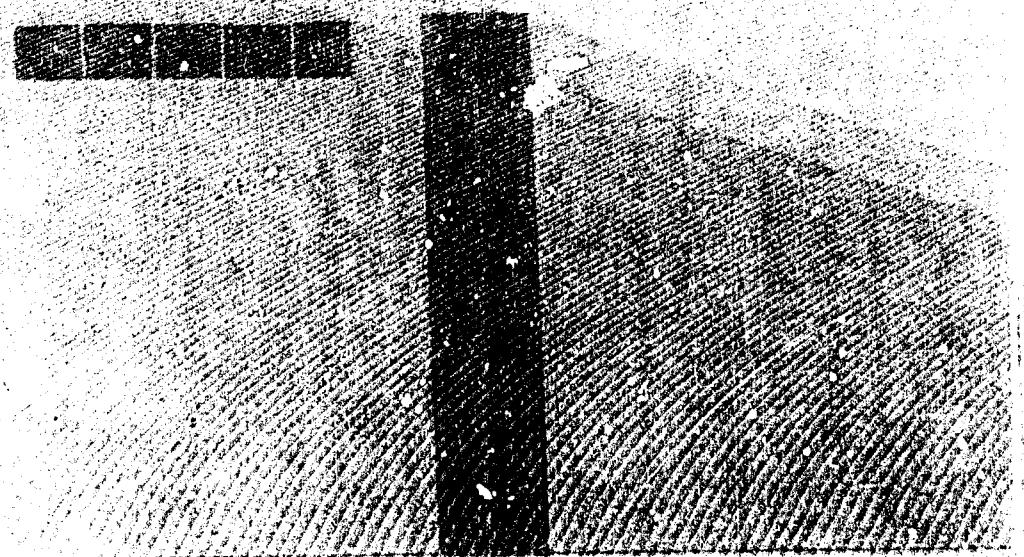


Table 6

ERRORS IN CALCULATED TGS ASSOCIATED WITH PARTICULAR GROUPS

TABLE 6

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ERRORS IN CALCULATED TGS ASSOCIATED WITH PARTICULAR GROUPS

UNLIMITED

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5. DRIC Code for Originator 7673000W	6. Originator (Corporate Author) Name and Location Royal Aerospace Establishment, Farnborough, Hants, UK		
5a. Sponsoring Agency's Code	6a. Sponsoring Agency (Contract Authority) Name and Location		

7. Title Calculation of the glass transition temperatures of linear polymers
Part 3 Evaluation of calculation relationships

7a. (For Translations) Title in Foreign Language

7b. (For Conference Papers) Title, Place and Date of Conference

8. Author 1. Surname, Initials Lee, W.A.	9a. Author 2	9b. Authors 3, 4 ...	10. Date June 1988	Pages 103	Ref. S
11. Contract Number	12. Period	13. Project	14. Other Reference Nos. Materials & Structures 233		

15. Distribution statement

(a) Controlled by - Head of Materials and Structures Dept

(b) Special limitations (if any) -

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16. Descriptors (Keywords) (Descriptors marked * are selected from TESI)

Polymers. Transitions. Glass temperatures. Calculation.

17. Abstract

Four equations, relating the structure of polymers in numerical form to their glass transition temperatures (T_g s), are evaluated using a large data set of 1179 polymers. Additive temperature parameters, for the relationship giving the best fit to the data, are tabulated which enable predictions to be made of many polymer T_g s outside the data set. These parameters also provide a measure of the relative effectiveness of groups in internally plasticising polymers.